TurboMass Software User's Guide

Release History

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Compatability

This software can be used with the TurboMass Gold or Clarus 500 Mass Spectrometer and the AutoSystem XL GC or Clarus 500 GC. In this *Software User's Guide*, we have used GC to indicate Clarus 500 GC or AutoSystem XL GC, and MS or mass spectrometer to refer to either the Clarus 500 MS or the TurboMass Gold instruments.

Using this Guide

The *TurboMass Software Guide* is a step-by-step guide for using TurboMass software. It is to be used in conjunction with the *Hardware Guide* and *Tutorial* manuals shipped with your instrument when setting up and performing runs on your Gas Chromatograph/Mass Spectrometer (GC/MS) System.

NOTE: This guide does not cover the installation and configuration of your computer. If you have purchased a complete system from PerkinElmer, the computer will already have been configured.

Chapters in this manual cover the following topics:

Chapter 1	**Introduction**	Software and hardware requirements.
Chapter 2	**Getting Started**	Navigating the main desktop and performing some common tasks.
Chapter 3	**TurboMass Overview**	Overview of the data acquisition process.
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Appendix B	**TurboMass Software Installation**	Reinstalling TurboMass software.
Appendix C	**TurboMass Quantify Calculations**	Presents methods for performing quantify calculations.
Appendix D	**Sample and Compound Table Output Fields**	Defines output table field options and formats.
Appendix E	**LIMS Import File Example**	An example of a LIMS file. Sample List for import.
Appendix F	**Environmental Reporting Calculations**	Equations showing the reporting calculations.

Conventions used in this Guide

This guide, designed for Windows users, assumes that you will be using a mouse or similar device to perform TurboMass operations. Many shortcut keys are listed on the TurboMass menus, and the documentation for your operating system can provide information about equivalent keyboard procedures. This section discusses capitalization, terminology, and the way that references are used in this guide.

- All menus, commands, and dialog option names appear with initial capital letters whether or not they are completely capitalized in the user interface. The names of keyboard items, such as the ENTER key, are capitalized. This will help you to distinguish these items from narrative or procedural text.

- Throughout the TurboMass documentation, the following terms are used to refer to program elements and the actions that you perform to carry out tasks:

  Click - The term *click* refers to moving the mouse pointer over a button or icon on the screen, and depressing the left mouse button.

  Select - The term *select* refers to highlighting an object or item or moving the cursor focus. Selecting an item prepares it for an action: for example, when you select text, it appears in reverse video. When you select a dialog option, you activate the option but the function is not carried out until you click **OK**, which closes the dialog and sometimes completes another operation.

  Enter or select - When you use the File Select or File Open dialog to open a file, the phrase "enter or select" is used to refer to the actions you can take to open that file. When you *enter* a filename, you type it in the File Name field exactly as it exists. When you *select* a file, you browse for it on your computer or your network. When you select a file, you will not introduce typographical errors.

- Unless otherwise indicated, the values in the illustrations of this manual are examples only. They are not intended to indicate the exact values you will see or to suggest the values you should use for a specific application.

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Getting Started

Starting TurboMass

To start TurboMass:

Double-click the desktop shortcut

OR

Use the Windows **Start** menu.

If TurboMass Security is enabled, the TurboMass Login window opens.

Enter your Logon Name and Password, and click **OK**.

The TurboMass menu bar will appear at the top of the display.

If you have trouble starting TurboMass, there may be a problem with your Security setup. See *Appendix A TurboMass Security* on page 659.

Quitting TurboMass

To terminate a TurboMass session, either click the Windows close box, or select **Exit** from the TurboMass **File** menu.

If data acquisition is in progress when you attempt to exit TurboMass, a dialog box informs you that the data will be lost, and asks if you still want to exit. If you click **Yes**, the acquisition stops, and the software shuts down. If you click **Cancel**, the acquisition continues.

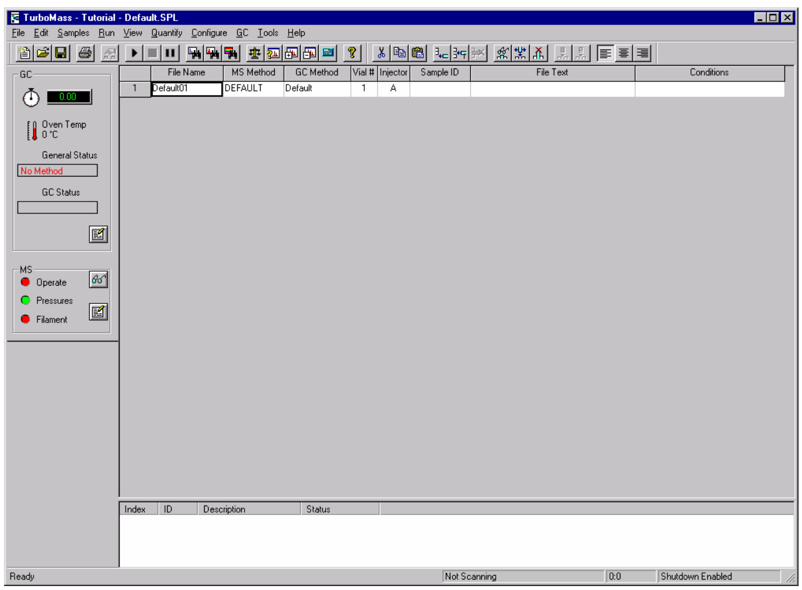
General Guidelines for TurboMass Operation

- Always use unique data file names within a Sample List.
- Always use unique names for Sample Lists before submitting them to a queue filled with other Sample Lists.
- Do not stop the Sample List while "General Status" says "Setting Up".
- Make sure the GC run is sufficiently long that the autosampler tower has stopped moving before the run is completed.
- If the GC autosampler tower has been manually moved, make sure it is returned to the "home" (full counter-clockwise) position before the next injection.

The TurboMass Top Level Window

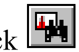
The TurboMass top level window includes features that allow you easily navigate through the software, work with files, and perform tasks.

- The menu bar includes options that allow you to access a variety of features. Menus include File, Edit, Samples, Run, View, Quantify, Configure, GC, Tools, and Help.
- The GC panel on the left side of the screen includes a run time indicated to display how long the acquisition method has been running, the Oven temperature, and status information.
- The MS panel below the GC pane displays the status of the mass spectrometer.
- The currently selected Sample List appears in the main pane.
- An Index of acquisitions queued on the mass spectrometer and the status of each appears on the lower portion of the screen.



The TurboMass Toolbar

The TurboMass toolbar includes buttons that allow you to quickly access a variety of common tasks and options. To see the function of a particular button, roll the mouse pointer over the icon to display a pop-up definition.

For example, to access Chromatogram from the toolbar, click .

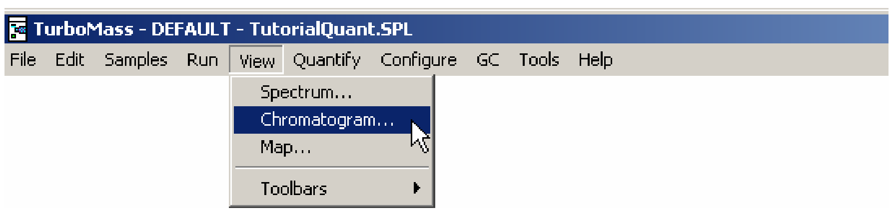
Accessing Menu Commands

All TurboMass menu commands are accessible by the mouse or keyboard commands according to standard Windows conventions.

For example, to select the Chromatogram:

Using the mouse From the TurboMass **View** menu select **Chromatogram** to open the Chromatogram application.

Using the keyboard Each top level menu will have one underlined letter, the "key letter." Press ALT+key letter to display a drop-down menu. For example, press ALT +V followed by C to open the Chromatogram application.



The sample list pane includes a context-sensitive menu that allows you to apply options to the queued samples. To access the drop-down menu, right-click an item or area. The following table describes the options:

Pause Process Right-click an entry and select this option to pause this entry.

Delete Process Right-click the Index of an entry and select this option to

delete the entry from the queue.

Priority Process

Right-click the Index of an entry and select this option to move this entry to the top of the queue.

Refresh Queue

If an entry has been deleted or prioritized, select this option to refresh the queue display.

Pause Queue

Toggle this option to pause/resume all acquisitions. A check indicates that a queue has been paused. The currently running entry will continue to completion, but no new acquisitions will be started. The queue can also be paused by selecting **Pause Queue** from the **Run** menu or by clicking .

Delete Queue

Select this option to delete all entries in the queue.

Pre-emptive Scheduling

This option allows priority processes to interrupt non-priority processes.

If this option is selected and a non-priority process is acquiring data, when a priority process is added to the queue, the current sample will be acquired, the current process will then be paused, and the priority process will start acquisition. When the priority process has finished acquiring data, the previous process will continue. If selected, a check will appear next to the process.

To open a recently used sample list select one of the four sample lists displayed at the bottom of the **File** menu.

The TurboMass Desktop

TurboMass uses a multiple window system that is controlled from the TurboMass top level window. Each component of the system, such as the Chromatogram display or the Tune page, has its own window and menu bar. These frames can be independently positioned, and in some cases resized. The different components can be linked together to allow easy data flow around the system. The desktop can be automated to provide a complete turnkey custom application.

When you exit TurboMass, the current layout is saved in the Username.ini file and reopened the next time you open TurboMass.

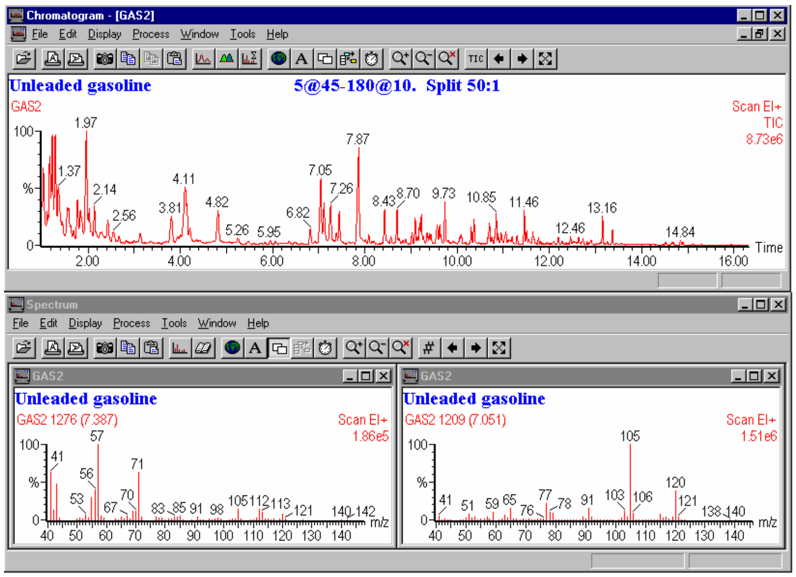


Figure 1 A TurboMass multiple window layout

Function Keys

The function keys can be configured by selecting **Options** from the Sample List **Tools** menu. On the **Processes** tab, use the **Add**, **Edit** and **Remove** buttons to change function key assignments. By default, the F1 key provides a link between the

TurboMass spectrum environment and the optional NIST library search program. Refer to the NIST manuals for instructions on using the NIST library search program.

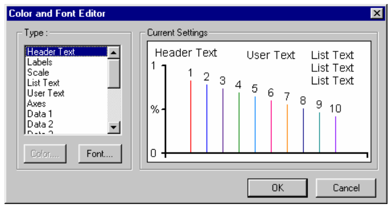
Other function keys can be assigned to other commands (.exe files).

Changing Colors and Fonts

The fonts and colors used to display information in TurboMass windows can be altered using the Color and Font Editor. To change TurboMass fonts or colors:

1. Select **Colors and Fonts** from the TurboMass **Tools** menu.

   The Color and Font Editor dialog is displayed.

2. Select a font **Type** from the list.

   The **Font** or **Color** button will become active as appropriate.

Select the appropriate button to enter the Font or Color editor

OR

Double-click a **Type** from the list to open the relevant editor

OR

Double-click a portion of the **Current Settings** spectrum to open the relevant editor.

Make any changes required to the fonts or colors of any part of the display.

Your changes will be reflected in the **Current Settings** spectrum display. This gives you the opportunity to experiment before making your changes permanent.

Click **OK** to exit the dialog.

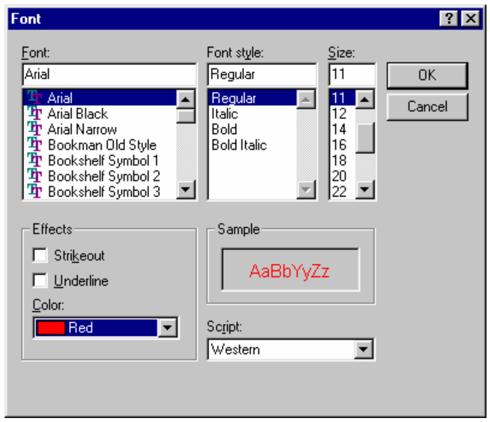
Any TurboMass displays affected by these changes are updated.

The Font Editor

The Font Editor allows the font, font style, font size, color, effects, and script to be changed. Any changes can be viewed in the **Sample** text.

To change fonts, select the required colors and fonts and click **OK**.

NOTE: *Selecting* **Cancel** *in the Colors and Fonts Editor will disregard these changes.*



To change data colors, select the required colors and click **OK**.

NOTE: *Selecting* **Cancel** *in the Colors and Fonts Editor will disregard these changes.*

The color editor displays 48 basic colors:

Data colors 1 to 5 are used for chromatogram traces and spectra.

Data colors 6 to 10 are used in the Map program.

Data color 5 is also used to set the color of tune peaks on the Tune page.

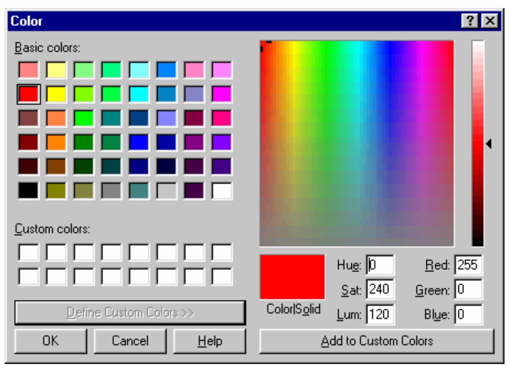
To define custom colors:

1. Click **Define Custom Colors** on the Color dialog.

2. To define the colors, either drag the cross-hairs and the arrow

   OR

   Enter **Hue**, **Sat**, **Lum**, **Red**, **Green** and **Blue** values until the required color appears in the **Color|Solid** field.



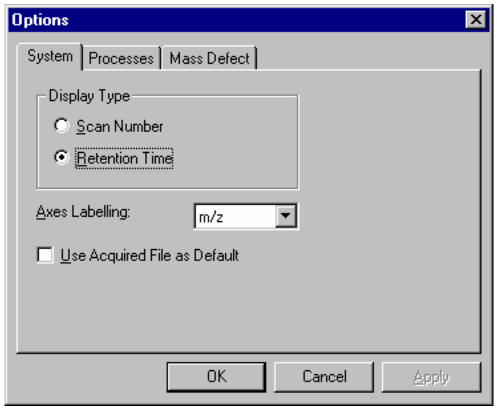
3. Click **Add to Custom Colors** to display the new color in one of the **Custom colors** fields.

4. Click **OK**.

TurboMass System Global Parameters

TurboMass includes an option that allows you to specify preferences that apply to a number of windows. These options are called TurboMass System Global Parameters. Rather than setting these parameters in every window, you can set the values at the top level, and the system will automatically apply the settings to all relevant windows.

To modify the System Global Parameters, select **Options** from the TurboMass **Tools** menu to display the Options dialog.



Display Type Select either **Scan Number** or **Retention Time**. This will determine the values entered to select spectra in Spectrum and Library.

Axes Labeling Select **Da/e**, **u/e** or **m/z** to determine axis labeling for spectral displays.

Da represents Daltons (previously called amu).

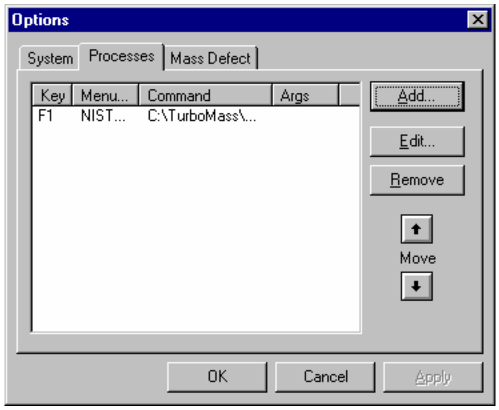
u represents atomic mass units.

e represents the elementary charge.

Use Acquired File as Default Select this parameter to always show the last acquired raw file when the Spectrum or Chromatogram windows are opened.

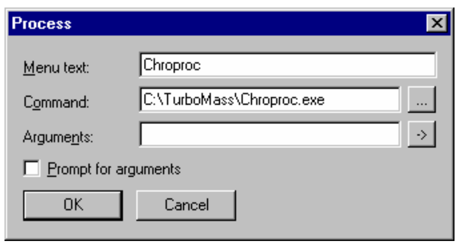
Processes

External processes can be added to the TurboMass **Tools** menu. Select **Options** from the top level **Tools** menu, and select the **Processes** tab.



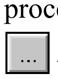
Adding a process

1. From the **Processes** tab, click **Add** to display the Process dialog.



2. Enter the text that will appear on the menu in the **Menu text** field.

3. Enter the process name and path in the **Command** field.

   Clicking  will open a browser to help locate the required executable program file.

4. If the process requires arguments that do not change, enter them in the **Arguments** field

OR

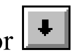
For arguments that are variable, select **Prompt for arguments**.

TurboMass will prompt you to enter the required information.

5. Click **OK**.

   Each process added to the list is assigned an unused function key as a shortcut to the process. This shortcut key is displayed in the **Key** field. To run the process, either select the process from the top level **Tools** menu or press the shortcut key.

Moving a process

Left-click the **Key** field of the process to be moved and click  or . Move buttons until the process is in the required position.

NOTE: *The shortcut keys remain in the same order so some processes may have a new shortcut key.*

Modifying a process

1. Select the key part of the entry you want to modify and click **Edit**.

2. Modify the required text, and click **OK**.

Deleting a process

1. Select the key part of the entry you want to delete and click **Remove**.

2. Click **OK**.

Mass Defect Correction

Mass Defect Correction can be used to improve quantification and library searches at higher masses. Select **Options** from the Sample List **Tools** menu. In the Options dialog, select the **Mass Defect** tab.

With the exception of carbon, the masses of all elements are non-integer. Some elements, such as chlorine and bromine, have larger deviations from integer than others. These high "mass defects" accumulate, and can cause mass misidentification, which leads to failed quantification and library searches at higher masses. You can specify a Mass Defect Correction value to apply a sliding window to correct for this mass defect. Mass Defect Correction can be applied post-run, so you do not need to reacquire your data files.

The *mass defect* is the difference between the exact mass of the ion and that calculated from the integer *nominal masses*. The mass defect is used in the mass calculation as:

nominal mass = (calibrated mass) - (mass defect)*(calibrated mass)

where:

nominal mass is what is displayed in Chromatogram or Spectrum

calibrated mass is from the FC-43 mass calibration file (mass defect $n = 0$)

mass defect is in mDa/Da

Carbon is defined as 12.00000... Da, or a mass defect of zero. All other elements are non-integer atomic weight. Chlorine, for example, is 34.9689 Da, a mass defect of -0.0311 Da, and bromine is 78.9183 Da, a mass defect of 0.0817 Da.

By the time you get to $C_{12}Br_{10}$, you get 933.1834 Da, instead of (12*12 + 79*10) = 934.0000 Da. The mass defect for this compound is thus -0.8166 Da. The mass defect correction is:

(934-933.1834)/934 = -8.743e-4 Da/Da = -0.8743 mDa/Da.

By this example, a measured mass of 933.1834 Da gives a nominal mass of:

933.1834 - (-8.743e-4)*933.1834 = 934 Da

TURBOMASS.INI

The TURBOMASS.INI file contains current settings for all TurboMass windows and dialogs. When a new user logs on, a new Username.ini file is created. Each time this user uses TurboMass, any changes to the current settings are saved to this file.

Selecting and Viewing Data

The Data Browser

The Data Browser lets you select a data file to work with. The Data Browser can be accessed from the TurboMass window by selecting **Open Data File** from the **File** menu, or from Spectrum, Chromatogram and Library programs by clicking  or selecting **Open** from the programs **File** menu.

The data file selected can be in any directory, on any disk, even a network disk. The browser can access the file header information for every data file and uses it to display the sample text information and scanning function information for a selected file. This allows you to find out what is in a data file without having to display a chromatogram or spectrum.

The Data Browser also holds the history information that gives you access to any processed data that have been derived from the original data, easing the management of processed data.

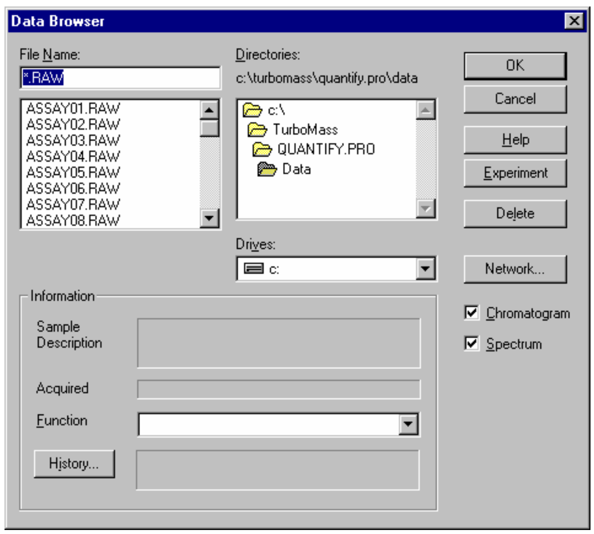


Figure 2 Data Browser

Selecting a new raw data file

In the **File Name** field, enter or select the name of the raw data file you require, and click **OK**.

If you do not see the name of the raw data file you want to work with, select a new drive or directory or double click an item in the File Name list.

Main Data Browser

The main Data Browser appears when you select **Open Data File** from the TurboMass top level **File** menu. It has the following two options that do not appear on the Spectrum or Chromatogram Data Browsers:

Chromatogram Automatically opens the Chromatogram window displaying the chromatogram of the new data file.

Spectrum Automatically opens the Spectrum window displaying the spectrum of the new data file.

Spectrum and Chromatogram Data Browsers

The Spectrum and Chromatogram Data Browsers appear when you select **File**, **Open** from Spectrum or Chromatogram. They have the following three parameters that do not appear on the Main Data Browser:

Add The data are added to data currently displayed as a new trace in the same window.

Replace The data replace existing data in the window.

New Window The data are displayed in a new window.

The Chromatogram Data Browser has an additional parameter that does not appear on the Main Data Browser:

Replace All If you are displaying the mass chromatograms for a number of selected masses and select this parameter, when the new file is opened, traces will be replaced by traces at the same masses.

Data Browser Fields

File Name Lists data files in the current directory and provides a field where you can enter or select a file name. The file name may include a path if required.

Directories Lists the directories available on the current drive.

Drives Lists the other available drives. These will include floppy disk drives and network drives when available.

Information Contains information relevant to the currently selected data file.

Sample Description Contains the sample description text obtained from the header of the currently selected data file. This will be information such as compound name and concentration that was entered during acquisition.

Acquired Contains the date and time of data acquisition.

Function Displays the acquisition function currently selected. The function description gives the function type, mass range and ionization mode.

To select a new function, click the arrow at the end of the Function field and left-click one of the Functions from the list.

History Contains the history of any processing that has been applied to the current data. When raw data are processed, for example, Refine or Combine, the processed data can be saved using the **Save Spectrum** command from Spectrum **File** menu. Selecting **History** in the History Selector dialog allows you to select one of the processed data files.

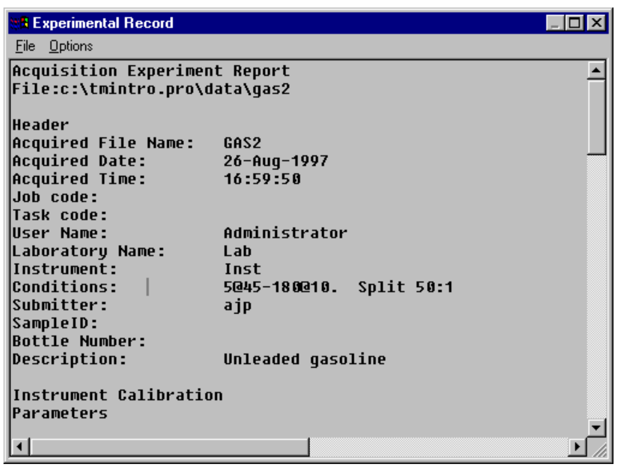
Experimental Record

The Experimental Record window displays information about the selected raw data file including:

- Raw data file header information such as sample description, acquisition date and time.
- Tune parameters, including the settings on the Tune page and instrument thresholds.
- Function description showing the functions set up in the Scan Functions window.
- GC information including the GC inlet position, vial number, run log, and GC method information.

Controlling the Experimental Record display

1. From the Chromatogram Data Brower, click **Experiment** to open the Experimental Record window.



2. From the **Options** menu, select the items that you want to be included in the experimental record display.

   When an item has been selected, a check mark will appear next to its name. The options available for inclusion in the experimental record display are **Header**, **Tune parameters**, **Function description** and **GC Information**.

Printing a report of the Experimental Record

Select **Print Report** from the Experimental Record **File** menu.

The currently displayed Experimental Record will be sent to the printer.

Deleting a Raw Data File

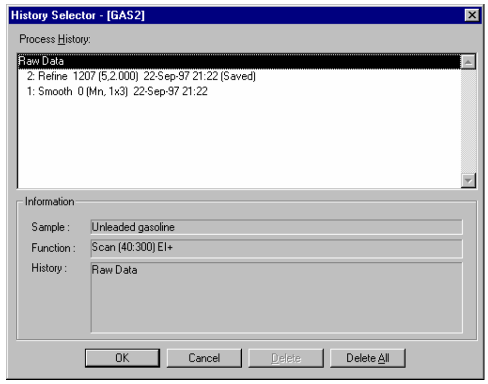
1. Select the data file you want to delete, and click **Delete**. A dialog will be displayed asking you to confirm that you want to delete this particular data file.

2. Click **Yes** to delete the file.

History Selector

The History Selector dialog allows you to access processed data. If no processed data are selected, raw data is the default. Processes are saved to disk when you select **Save spectrum** from the Spectrum **File** menu.

The History Selector also allows you to delete from disk processes that are no longer required.



Process History Displays the full history of all saved processes with the original raw data at the top of the tree.

Processed data that have been derived from previously processed data are indented to show the relationship to those data. Each process is labeled with a unique identification number and the time and date when it was created. This aids differentiation of similar processes.

Sample Displays sample description text obtained from the header of the currently selected data file.

Function Displays a description of the currently selected function.

History Displays full history of the currently selected process. The history starts with raw data at the top of the list and describes each processing step made to reach the current process.

OK Exits the History Selector using the current selection.

Cancel Exits the History Selector defaulting to the original selection.

Delete Deletes the currently selected process from the process history tree.

Delete All Deletes all processes belonging to the current data file function.

Displaying processed data

1. Select the relevant raw data file in the Data Browser dialog, and click **History**. The History Selector dialog is displayed.
2. Select the required processed data in the **Process History** list and click **OK**.
3. Click **OK** in the Data Browser dialog.

Processed Data Labels

Each of the processed data labels is followed by a series of letters and numbers that describe the parameters used during the process:

Refine Rf (n1, n2)

Rf Refined spectrum

n1 Refine window in scans

n2 Refine noise level

Combine Cm (n1:n2 - (n3:n4 + n5:n6) x n7)

Cm Combined spectrum

n1:n2 Average range start and end values

n3:n4 First subtract range start and end values

n5:n6 Second subtract range start and end values

n7 Subtract range multiplication factor

Smooth Sm (s1, [n1x], n2)

Sm Smoothed data

s1 Smooth type (Mn – mean, Md – median, Sg – Savitsky Golay)

n1x Number of smooths (not for median)

n2 Smooth window. TurboMass requires that you enter an estimate of the width of the raw data peak at half height in Daltons, and uses this to calculate the width of the smoothing window. See "Spectrum" for the rule used for this calculation.

Subtract Sb (n1, n2)

Sb	Spectrum which has been baseline subtracted
n1	Order of polynomial which has been fitted to baseline
n2	Percentage of data points which lie below baseline

Center Cn (s1, n1, [n2], s2)

Cn	Centered data
s1	Centering method (Top – highest point on peak, Med – Median of peak, Cen – centroid of peak)
n1	Peak width at half height
n2	Topmost percentage of peak used to calculate centroid
s2	Method used for calculating peak intensities, height 'Ht' or Area 'Ar'

Using Explorer to work with Multiple Data Files

It is also possible to use Windows Explorer to open several TurboMass data files at once and display them in Chromatogram or Spectrum.

Opening multiple data files

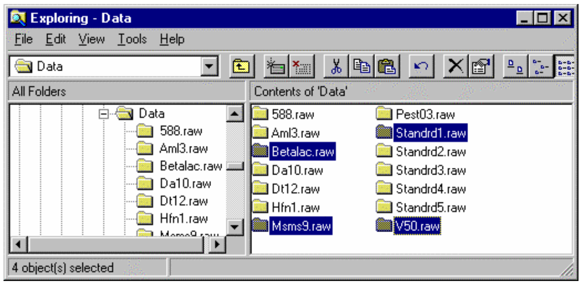
1. Open the Windows Explorer and the TurboMass Chromatogram or Spectrum application, and arrange the windows so that both are visible.

2. Select the TurboMass data files you want to view in the right side of the Explorer window.

3. Select more than one file by holding down the CTRL key while you click the files.

4. Drag the files into the Chromatogram or Spectrum window.

   The Chromatogram or Spectrum window will be redisplayed showing the first function in each data file as a separate trace.



Deleting multiple data files

1. Open Windows Explorer.

2. Select the TurboMass data folders you want to delete in the right side of the Explorer window.

3. Select more than one folder by holding down the CTRL key while you click the folders

   OR

   Select a block of folders by clicking the first folder in the block and then holding down the SHIFT key while you click the last folder in the block.

4. Press DELETE.

   You will be prompted to confirm that you want to remove the folder and move its contents to the Recycle Bin.

5. Click **Yes** to continue.

NOTE: *Files sent to the recycle bin are not deleted from the system; they will stay in the recycle bin until you delete or retrieve them from there.*

Projects

TurboMass comes with predefined projects: Default.pro, TutorialQuant.pro, TutorialReports.pro, Tutorial_VOA.PRO, and Tutorial_SVOA.PRO. All data are stored in the Default.pro project until a new project has been selected or created.

All TurboMass data storage is organized into projects. When you create a TurboMass project, TurboMass creates a new directory called *ProjectName*.pro and the following sub-directories:

AcquDB	Acquisition settings files
CurvedDB	Quantify calibration curves
Data	Raw data files
MethDB	Quantify methods
PeakDB	Peak lists
QualDB	Environmental Library Search results
SampleDB	Sample lists

Creating a new project

1. Select **Project Wizard** from the TurboMass **File** menu.
   The Create project dialog is displayed.

2. Enter a **Project name** and **Description** in the appropriate fields.
   A default location, for saving the project to, appears in the location field.

3. To save the file to a different location, enter a new file name into the field

   OR

   Click **Browse** and select a file from the dialog displayed.

4. Click **Next** to display the next page.

5. Select one of the following as appropriate: Create New Project, Create Using Current Project As Template or Create Using Existing Project As Template.

   If **Create Using Existing Project As Template** is selected, the **Browse** button will be enabled. Click **Browse** to display the Select Existing Project dialog allowing you to select an existing project to use as a template.

   If **Create Project Using Current or Existing Project** is selected, all files in Acqudb, Methdb, and Sampledb are copied into the new project. If an existing project is not chosen as a template, all subdirectories will be empty.

6. To create the new project, click **Finish**.

   Clicking **Back** will display the previous page allowing changes to be made. Clicking **Cance**l will discard all information and exit the Project Wizard.

7. For TurboMass to create a new project it must close any TurboMass applications that are currently running. If you are currently running any of the TurboMass applications such as Spectrum or Chromatogram, a message will appear informing you that all applications will be closed. Click **Yes** to close any opened applications, and create the new project.

   All new data files, sample lists, peak lists, quantify method files and quantify calibration curves will be saved in this project until you change to a new project.

NOTE: *Space on drive C: is normally restricted. It is often useful to place data on other local drives (for example, d: or e:).*

Opening an existing project

1. Select **Open Project** from the TurboMass **File** menu.

2. Double-click one of the projects in the list, select one of the projects in the list, or enter your project name in the **Project Name** field.

3. Click **OK**.

   For TurboMass to change to a new project it must close any TurboMass applications that are currently running. If you are currently running any of the TurboMass such as Spectrum or Chromatogram, a message will appear informing you that all applications will be closed. Click **Yes** to close any open applications and change to the new project.

Directory Structure

When TurboMass is opened, a number of default folders will be created that contain information for different parts of the application. Files can be opened from, and saved to, any location that you specify, but TurboMass will look in the default folders for the information first. The following is a list of folders created in the TurboMass directory.

Folder Name	Type of information stored in the folder
IdenDB	Libraries against which searches are performed. Mass Spectral, NIST and user defined libraries
Macro	Macros
Ref	Peak list information for Calibration reference files
Shutdown	Shutdown parameters. MS methods for startup before and shutdown after acquisition
StructDB	Library chemical structures

The following table lists the folders that are created within projects:

Folder Name	Type of information stored in the folder
AcquDB	Acquisition defaults and saved Tune page settings, calibrations etc. Inlet method files
CurveDB	Quantify calibration curve data
Data	Raw data files
PeakDB	Peak list data
MethDB	Quantify methods
QualDB	Results of Tentatively Identified Compound (TIC) searched
SampleDB	Sample Lists

When a new version of TurboMass is opened, all files which are no longer compatible with the new version are stored in subfolders called Old. For example, old method files will be in the Old subfolder of the MethDB folder. These files can still be used with older versions of TurboMass but should not be used with the new version.

Data File Structure

Data acquired from the mass spectrometer are saved into data files on the computer's hard disk. These data files may contain more than one acquisition function and may also contain processed data derived from the original raw data, for example, refined spectra.

All files are acquired to the data directory of the current project. For example, if the file name is specified as test2 then the data files are stored in the directory c:\TurboMass*currentproject*\data\test2. If the data file contains 2 acquisition functions and 2 sets of processed data then the directory listing will be as follows:

_Header.txt	Data file header information
_Funcs.inf	Information on MS functions acquired
_history.inf	Information on how data has been processed
_expment.inf	Experimental record information
_Func001.dat	Data file for first function (one for each function)
_Func001.idx	Data file index for first function
_Func002.dat	Data file for second function
_Func002.idx	Data file index for second function
_inlet.inf	Information on GC method
_proc001.dat	First processed data file (one for each process)
_proc001.idx	Index for first processed data file
_proc002.dat	Second processed data file
_proc002.idx	Index for second processed data file
_Tcfunc1.raw	Data files from the first conventional GC detector
_Tcfunc2.raw	Data files from the second conventional GC detector

Displaying Spectra

There are several ways in which you can ask to display the Spectrum window. The two most common ways are selecting **Spectrum** from the TurboMass **View** menu or, double-clicking the Chromatogram window.

Selecting a spectrum using the TurboMass menu

➢ Select **Spectrum** from the **View** menu.

The spectrum displayed will be the current default spectrum (this will be either the last spectrum viewed, or, if acquisition is in progress, the last spectrum acquired). If the Spectrum window is already on display, it becomes the current window.

If whole rows are selected in the Sample List editor, spectra from the data files represented by these rows will be displayed.

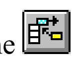
Selecting a spectrum from Chromatogram

➢ Double-click the chromatogram at the retention time of interest.

The spectrum displayed will be the spectrum closest in retention time to the position where the mouse was clicked.

If the Spectrum window is already on display, the selected spectrum will either be added to the one currently on display

OR

Will replace the one currently on display if the  Spectrum toolbar button is activated

OR

Will be displayed in a new document window of its own if the  Spectrum toolbar button is activated.

Removing spectra and document windows

- To remove a particular spectrum, select the spectrum to make it the currently selected spectrum, and press DELETE.

  Click **OK** to confirm the deletion.

- To close a particular Spectrum window, click the Windows close button ☒.

Displaying Chromatograms

Like spectra, there are several ways in which you can display the Chromatogram window. The two most common ways are selecting **Chromatogram** from the TurboMass **View** menu, and double-clicking the Spectrum window.

Selecting chromatograms from Chromatogram

Select **Chromatogram** from the **View** menu.

The chromatogram displayed will be the Total Ion Current (TIC) chromatogram of the current data file. If the Chromatogram window is already on display, it becomes the current window.

If whole rows are selected in the Sample List editor, Chromatograms from the data files represented by these rows will be displayed.

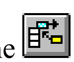
Selecting chromatograms from Spectrum

➢ Double-click the spectrum at the mass of interest.

The chromatogram displayed will be the mass chromatogram of the mass indicated by the click.

If the Chromatogram window is already on display, the selected chromatogram will either be added to the one currently on display

OR

Will replace the one currently on display if the  Chromatogram toolbar button is activated

OR

Will be displayed in a new window of its own if the Chromatogram toolbar button is activated.

Removing chromatogram traces and windows

- To remove a particular chromatogram trace, select the trace to make it the currently selected trace, and then press DELETE.

  Click **OK** to confirm the deletion.

- To close a particular chromatogram window, click the Windows close button ☒.

The Header Editor

The Header Editor is used to determine the information displayed in the header for each of the TurboMass windows.

The TurboMass Window Header can be thought of as a table that has six rows and three columns. Various pieces of information can be displayed in the header including your own text. Information can be displayed in lines 1 to 6. On each line, information can be displayed in three positions: left, center, or right.

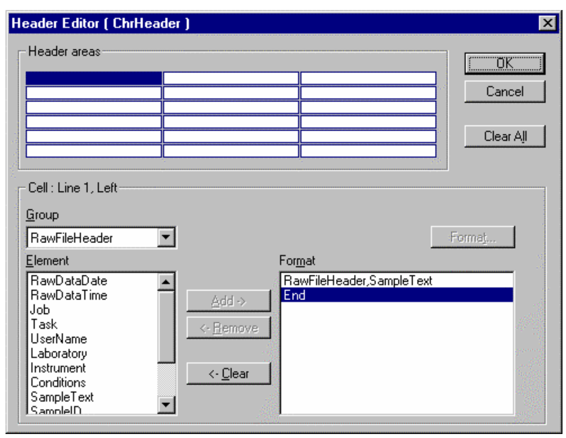
There is a graphical representation of the current header at the top of the Header Editor dialog. The Header Editor areas that are currently displaying information are shaded in gray. A maximum of eight areas can be used at one time to display header information.

Determining the Header Information in a TurboMass Window

- To open the Header Editor dialog, in most TurboMass windows double-click the Window header

  OR

  Select **Header** from the Display View dialog.



Adding information to the displayed header

1. Select the Header areas in which you want to display information.

2. Select the Group, from the drop-down list, that contains the information you want to append to the displayed header.

3. Select the information required in the Element list.

4. Select the field before which you want to insert the information in the Format field, and click **Add**.

   To add information at the end of the currently displayed information, select **End** and click **Add**.

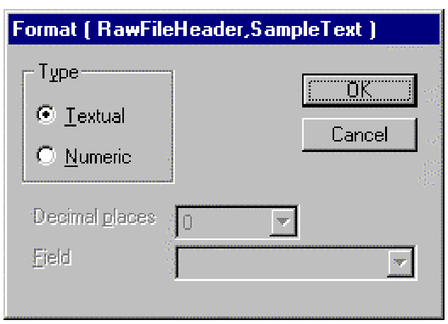
5. To add your own text to the header, select [Text] in the **Element** list and click **Add**.

   The User Text dialog is displayed.

6. Enter your text, and click **OK**.

   Your user text will be shown in the **Format** list and will be displayed in the header when you exit the Header Editor dialog.

7. If you want to format the information in the header, select the relevant field in the **Format** list, and click **Format**.

   For numeric information you can select the number of **Decimal places** displayed in the 0 to 6 range. Some Elements have sub-elements that may be selected by the **Field** list.

8. Repeat steps 1 to 6 as required.

   A maximum of eight areas can be used at one time to display header information.

9. Click **OK** to exit and save the changes.

NOTE: *If the information in one of the Header Editor areas overlaps another area, the overlapped area will not be displayed.*

Removing information from the displayed header

1. Select the **Header areas** from which you want to remove information.

2. To remove a single field, select the information you want to remove in the **Format** list and click **Remove**

   OR

   To remove all the information from one Header Editor area, select the area and click **Clear**

   OR

   To remove all information from all Header Editor areas, click **Clear All**.

3. Repeat steps 1 and 2 as required.

4. Click **OK** to exit and save the changes.

Printing Data

TurboMass prints data using the Windows Print Manager, so any printer supported by your Windows operating system can be used with TurboMass. All of the operations involved in setting up your printer are controlled by the Windows Operating System and will be described in the documentation that accompanied that. The only TurboMass specific procedures to learn are those involved in selecting what to print.

You can select the printer that you want to use and specify printer setup by using the **Printer Setup** command found in each TurboMass **File** menu, or by using the Windows Print Manager.

Many of the TurboMass Windows have Print buttons on the toolbar.

 Prints current window in portrait format.

 Prints current window in landscape format.

Printing a Specific TurboMass Window using the Menu

1. To print a specific TurboMass window using the menu commands, select the window you want to print, and then select **Print** from the window's **File** menu.

2. Select **All Windows** to print all document windows on display

   OR

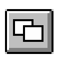
   Select **Current Window** to print only the currently selected document window.

Trace Width allows you to specify the thickness of the line used to print chromatogram traces or spectral peaks. **Trace Width** can be set to values between 1 and 5; a higher value will give a thicker line.

Print All Colors Black will map all the colors in the TurboMass display (except white) to black. This option is useful when using black and white printers.

Window Commands

Most of the TurboMass program windows have a top level menu command called **Window** that contains the standard Windows commands. Those specific to TurboMass are described here.

Toolbar Button	Menu	Function
	Window list	Window list gives a list of available windows. The currently active window has a check mark next to its name. Selecting another window will make that the currently active window. In the case of Spectrum and Chromatogram this becomes a list of the traces displayed in each window.
	Window New Trace Replace Trace	Choosing this option causes each subsequent trace to replace the currently selected trace.
	Window New Trace New Window	Choosing this option causes each subsequent trace to be displayed in a new window.
	Window New Trace Add Trace	Choosing this option causes each subsequent trace to be added to those displayed in the current window.

Getting Help

The TurboMass Help system contains detailed information on how to use TurboMass.

TurboMass Help can be accessed either from the TurboMass top level menu or from any of the TurboMass program windows.

If you enter Help from the TurboMass top level menu, you will be given a general index of topics covering the whole of TurboMass. If you enter TurboMass Help from one of program windows, you will be given help on that particular topic. For example, if you select **Help** from Spectrum, you will be given Help on Spectrum. TurboMass Help also allows you to search for Help on a specific topic or keyword.

For more information on using Windows Help systems, select **Using Help** from the **Help** menu on the TurboMass window. This topic gives detailed instructions on how to use Windows Help systems.

The About Box

The About TurboMass box gives you information about TurboMass, including the version number.

TurboMass Overview 3

This chapter describes how to use the TurboMass data acquisition system. It gives an overview of how to use TurboMass, including mass spectrometer and GC setup, method development, data acquisition, and data manipulation.

For specific information on how to perform your first run using your mass spectrometer system, refer to the *User's Tutorial* supplied with the mass spectrometer.

Starting TurboMass

1. To start TurboMass, double-click the TurboMass icon on the Windows desktop.

   If TurboMass Security is enabled, the TurboMass Login dialog will be displayed.

2. Enter your Logon Name and Password.

   TurboMass will start and communications with the instrument will be initialized.

Configuring the Inlet System

1. Select **Select Inlet Interface** from the Sample List **Configure** menu, and select your interface.

2. Configure your GC as described in the GC portion of the documentation.

Preparing the Mass Spectrometer for use

Prepare the mass spectrometer for operation as described in the *Hardware Guide* for your mass spectrometer.

If in a vented state, it should be pumped down. Then switch it into the Operate mode.

Tuning the Mass Spectrometer

The instrument must be tuned to obtain the best conditions for ionization according to the instructions in the *Hardware Guide* for your mass spectrometer

Calibrating the Mass Scale

- The mass scale must be correctly calibrated so that the masses reported for acquired data are correct.

  Calibration of the mass scale involves introducing a reference compounds into the system, acquiring initial data, and then comparing the result with the expected masses for the reference compound. A calibration curve is produced and used to correct for any errors in the mass scale.

Setting up your GC

- Set up your GC configuration and develop your GC method.

Developing your Mass Spectrometer Method

- Develop your mass spectrometer method for scanning the system (referred to as a Function) in the TurboMass Function List editor.

Setting up your Sample List and acquiring Initial Data

1. Specify your list of samples to be introduced into the system by manual or autosampler injection.

   Your sample list may contain a single sample or a number of samples.

2. Start your run to acquire data to be used for qualitative analysis or quantification method development.

Developing your Quantification Method

If you are performing quantitative analysis, develop a peak detection and location method based on the results of your initial data acquisition in the TurboMass Quantify application.

Developing your Qualitative Method

This is a dataset you can specify in each row of the sample list to generate reports that do not make use of the quantitative results.

Acquiring Data based on your Method

You can now acquire data and apply your quantification method parameters.

Monitoring Data Acquisition

The progress of the acquisition can be monitored by viewing the data acquired in real time using the Spectrum or Chromatogram displays.

Manipulating your Data

You can manipulate your data in many ways using the TurboMass Chromatogram, Spectrum, Map, Quantify, Strip, and Combine functions.

Reporting your Data

You can use supplied templates or create your own templates using the Communiqué template designer to generate custom reports.

Instrument Data Thresholds

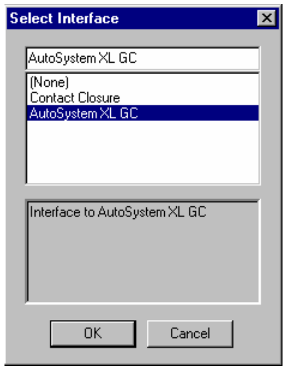
4

Selecting the Inlet System

Before you acquire data, you must first configure the software to support the inlet system selected. You do this from the Select Interface dialog, which displays the available inlet systems.

1. Select **Select Inlet Interface** from the Sample List **Configure** menu.

   The Select Interface dialog is displayed.

2. Select your interface.

   The list of inlet options that appears in the Select Interface dialog reflects the inlet system selected when TurboMass was installed. If, at a later date, you add a new inlet system or change one of your existing inlets you may need to reinstall TurboMass to gain access to the control software for the new inlet system.

3. Select your choice for an inlet to use and click **OK** to reconfigure the software to reflect the new inlet system.

   Once you have selected the inlet system, TurboMass will give you access to the parts of the acquisition system that are appropriate to the inlet selected and the Tune application.

Setting Instrument Data Thresholds

TurboMass has Instrument Data Thresholding parameters that allow you to control how the system preprocesses data before they are sent to the host computer.

Instrument Data Thresholding allows you to specify the type of data you want to acquire and save to disk, and which type of data you want to discard. Limiting the amount of data stored on disk can be particularly desirable when acquiring continuum data and doing long GC runs. Additional options allow you to set the SIR Baseline Level, the ion counting threshold, spike removal and zero baseline offset.

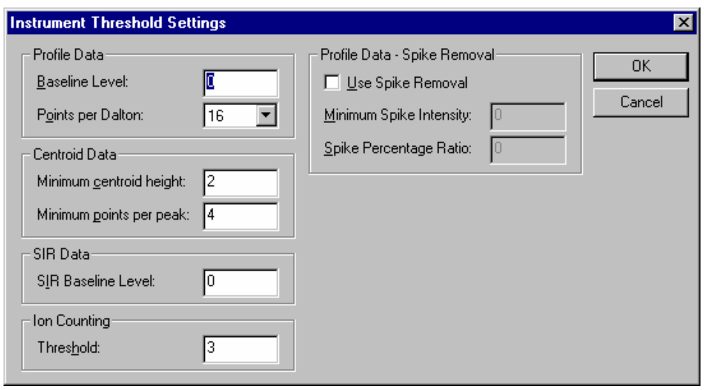
Setting Data Thresholding Parameters

Changing data thresholding parameters

1. Display the Tune page by clicking  in the **MS** section of the instrument status panel in the TurboMass top level window.

2. On the Tune page, select **Instrument Threshold Settings** from the **Options** menu.

   The Instrument Threshold Settings dialog appears.



3. Set your parameters.

Profile Data

While not normally used for GC/MS, TurboMass can collect **Profile Data** that shows mass peak shapes, as in Tune. The profile data parameters let you control the amount of data collected during a continuum data acquisition. By default, TurboMass collects one data point every 16th of a Dalton. For example, if you scan from mass 50 to mass 1200, you will collect and save 18,400 data points per scan. As each point requires 6 bytes of disk space, every scan will require 55.2 KB of disk space in this example. So, if you use this type of scanning in conjunction with chromatography, the data file sizes will grow to be enormous. In addition to the disk space issue, collecting this amount of data puts a heavy demand on the transputer system, which will ultimately affect the scan rates at which you can collect data.

The ability to use a threshold with continuum data is therefore highly desirable as it lets you disregard data that is noise yet save the complete peak profile for the "real" data. The use of a threshold with continuum data retains the information in the data while reducing disk space requirements.

Baseline Level	Raises or lowers the baseline to see more or less noise. The **Baseline Level** parameter sets the baseline position above zero when **Ion Counting Threshold** is not enabled (set to zero). The **Baseline Level** parameter is typically set to **0**. If you want the baseline to appear higher, increase the value of the **Baseline Leve**l parameter. You can use a negative **Baseline Level** value to reduce the amount of noise seen and apply thresholding to 1/16th Dalton type samples. This thresholding occurs after ion counting and therefore has a less significant effect. If you want to see more noise, use a positive value. Do not use a positive **Baseline Level** value with **Ion Counting Threshold**.
Points per Dalton	Can be set to one of three values, 4, 8 or 16. Selecting 8 points will allow you to acquire data twice as quickly as selecting 16, and will (in continuum mode) result in data files that are approximately half as big as those acquired at 16 points per Dalton. Selecting 4 points will allow you to acquire data twice as quickly as selecting 8, and will result in data files that are approximately half as big as those acquired at 8 points per Dalton. Acquiring data at 16 points per Dalton gives the greatest possible resolution. Acquiring data at 4 points per Dalton gives data with a smoothed appearance.
Centroid Data	For centroided data (the type most commonly used for GC/MS), there are two parameters that you can set.
Minimum centroid height	The Intensity level below which peaks detected will be ignored. Typical value is 2. [Should not be changed.]
Minimum points per peak	The minimum mass peak width. Typical value is 10 for 16 points per Dalton. [Should not be changed.]

NOTE: *Data is acquired according to the* **Profile Data** *criteria before it is centroided.*

SIR Data - SIR Baseline Level

Used when **Ion Counting Threshold** is not enabled (set to zero). **SIR Baseline Level** sets the baseline position above zero. The **SIR Baseline Level** is typically set to **1**. If you want the baseline to appear higher, increase the **SIR Baseline Level** value.

Ion Counting Threshold

Sets the intensity level below which a data point will be ignored. The **Ion Counting Threshold** can be set to values between 0 and 25; the higher the value, the more data will be discarded.

NOTE: *To disable the* **Ion Counting Threshold**, *set the value to zero. If you want to use the* **Ion Counting Threshold***, a value of 3 is suitable for most data. If you are performing trace analysis or looking at small isotope peaks, a value from 1 to 3 may be more appropriate. If you are only looking at large peaks, you can save disk space with a higher number.*

This threshold is applied to all acquisitions, regardless of scanning mode. It is also the most significant of all of the data manipulation variables because it is the one applied first to the raw data.

When an acquisition is started, the instrument performs a "prescan" with the ion beam turned off so that the electronic noise level of the acquisition system and its standard deviation can be measured. The **Ion Counting Threshold** level that you enter is multiplied by the standard deviation of the noise to determine the intensity level to be used. If you set a value of zero, the intensity level is set so that it sits in the middle of the noise range, which would mean that roughly half of the noise data will be acquired. If you set a value of 20, the threshold would sit well above the noise level, so very little noise data will be acquired. Conversely, a value of 1 would place the threshold just above the noise so almost all of the data will be acquired.

NOTE: When using an **Ion Counting Threshold**, you should set the **SIR Data SIR Baseline Level** and the **Profile Data Baseline Level** to zero.

The value of the **Ion Counting Threshold** should be set such that background noise is removed without significantly reducing the intensity of the smallest peaks of interest.

NOTE: *When using an* **Ion Counting Threshold***, you should set the* **Profile Data Baseline Level** *and* **SIR Data SIR Baseline Level** *to zero.*

Profile Data – Spike Removal Spikes are distinguished from real data by the fact that spikes are very narrow and also very intense when compared to their immediate neighbors. Data points that are determined to be spikes are removed by setting the value of each spike data point to the average of its immediate neighbors.

NOTE: *The use of* **Spike Removal** *does involve some additional processing during acquisition, which will reduce the maximum achievable acquisition rates by approximately 30 %.*

Use Spike Removal Select this checkbox to perform spike removal during an acquisition.

NOTE: *Spike removal will not be reflected on the Tune page.*

Minimum Spike Intensity Sets the intensity threshold below which spikes will be ignored. Take this value from the Tune page intensities. A very low intensity signal may include single ion events that can be combined to produce significant peaks. For this type of data, you should set the **Minimum Spike Intensity** to a suitable value such that these single ion events are not discarded as spikes.

Spike Percentage Ratio Sets the ratio used to determine whether a data point is a spike. This determination is made by comparing the data point to its immediate neighbors.

If the **Spike Percentage Ratio** is set to 30 %, then if at 30 % of its full intensity the data point is still more intense than both its immediate neighbors, it will be regarded as a spike. To express this as a ratio, the maximum allowed intensity ratio between a data point and its immediate neighbors is 3:1.

Spike Percentage Ratio set to 50 % is equivalent to a ratio of 2:1.

Spike Percentage Ratio set to 20 % is equivalent to a ratio of 5:1.

The following examples show the effects of changing the **Baseline Level** and **Ion Counting Threshold** parameters. A series of acquisitions were done using Heptacosa (FC-43, PTA, PFTBA) and acquiring continuum data. Each data file contains 18 scans. The data file AB0000 is not thresholded; both **Baseline Level** and **Ion Counting Threshold** were set to zero.

This first example shows the effect of increasing the **Baseline Level** parameter:

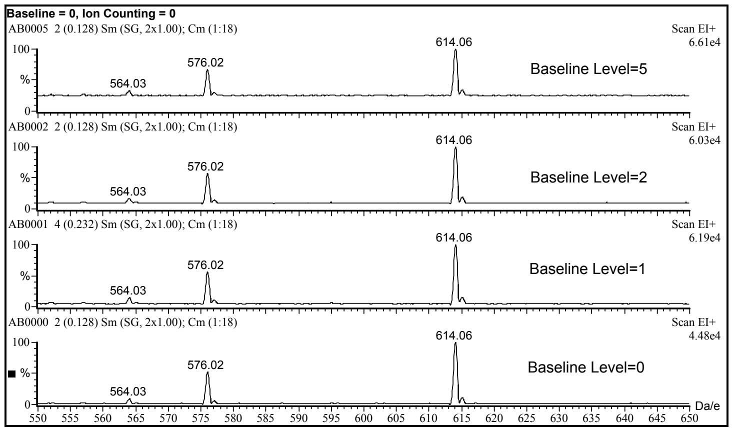


Figure 3 Effect of increasing Baseline Level on Heptacosa spectrum

The second example shows the effect of increasing the **Ion Counting Threshold** on a part of the spectrum that contains only background noise. The bottom trace was acquired with the **Ion Counting Threshold** set to zero. For subsequent traces, the **Ion Counting Threshol**d was set to 1, 2, 4, 6 and 25. As the **Ion Counting Threshold** is increased the amount of noise stored is reduced, the normalizing intensity value at the top right corner of the trace is also reduced.

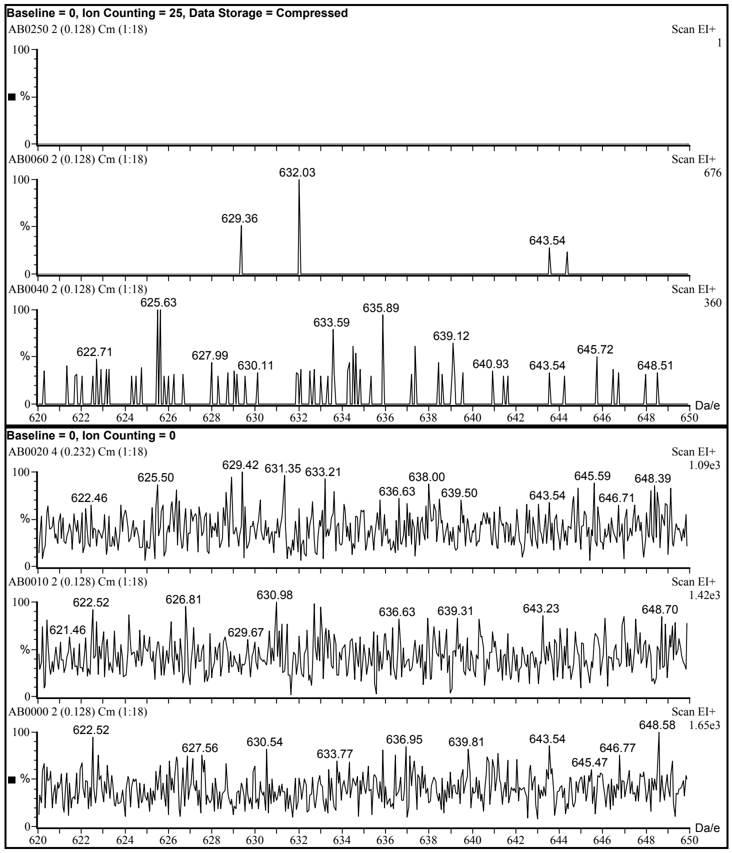


Figure 4 Effect of increasing Ion Counting Threshold on noise in Heptacosa spectrum

The value of the **Ion Counting Threshold** should be set such that background noise is removed without significantly reducing the intensity of the smallest peaks of interest.

The following example shows the effect of increasing the **Ion Counting Threshold** on a part of the spectrum that contains a low intensity peak. As the **Ion Counting Threshold** is increased beyond a certain value, the peak becomes narrower, and its

intensity is reduced as the thresholding rejects part of the genuine signal. In this case an **Ion Counting Threshold** value of 4 would be suitable.

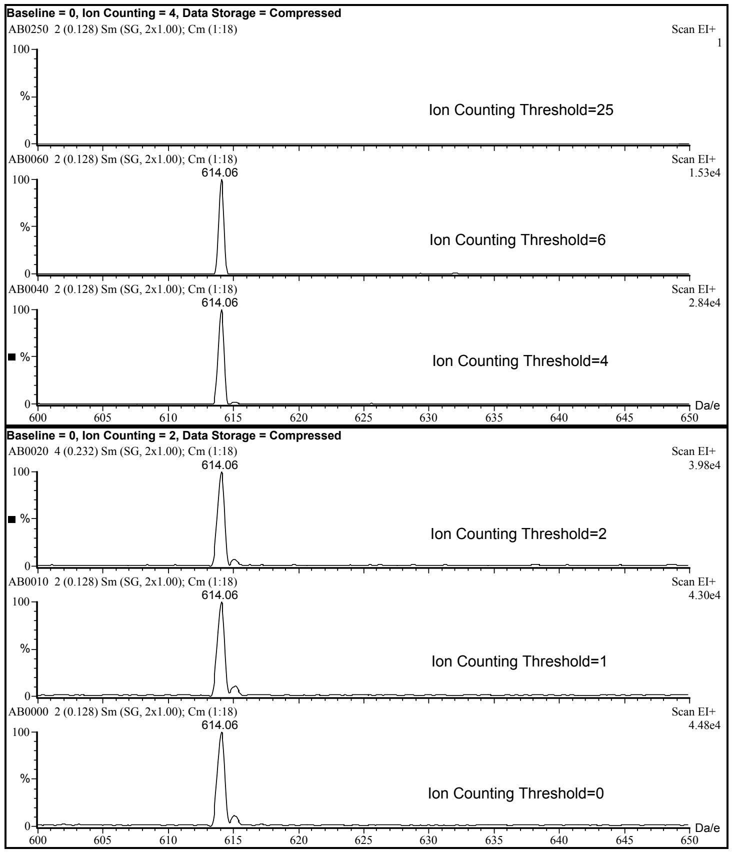


Figure 5 Effect of increasing Ion Counting Threshold on low intensity peak in Heptacosa spectrum

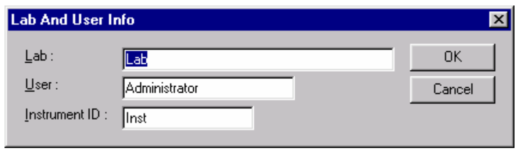
Changing Lab and User Information

TurboMass can save management information with a data file. The information saved is Laboratory Name, Instrument Identification and User Name. This information is entered into the Lab and User Info dialog.

This information will be stored with any data that are acquired and can be displayed as part of the header information of a chromatogram or spectrum when displayed or printed.

1. On the Tune page select **Instrument Name** from the **Options** menu.

   The Lab and User Info dialog appears.

2. Make required changes to the information.

3. Click **OK**.

Communications Status and Diagnostics

Communications Status

Select **Communications Status** in the Tune **Options** menu. A dialog indicates if the computer and the TurboMass instrument are in communication and the number of hours. The version of the communications protocol software is displayed.

In this dialog, clicking **Reboot** will download the communications protocol from the computer to the TurboMass instrument. This is used only for service diagnostics purposes.

When done, do not close the System Manager dialog. Click **Hide** to return to the Tune page view. Do not click **Exit**.

Diagnostics

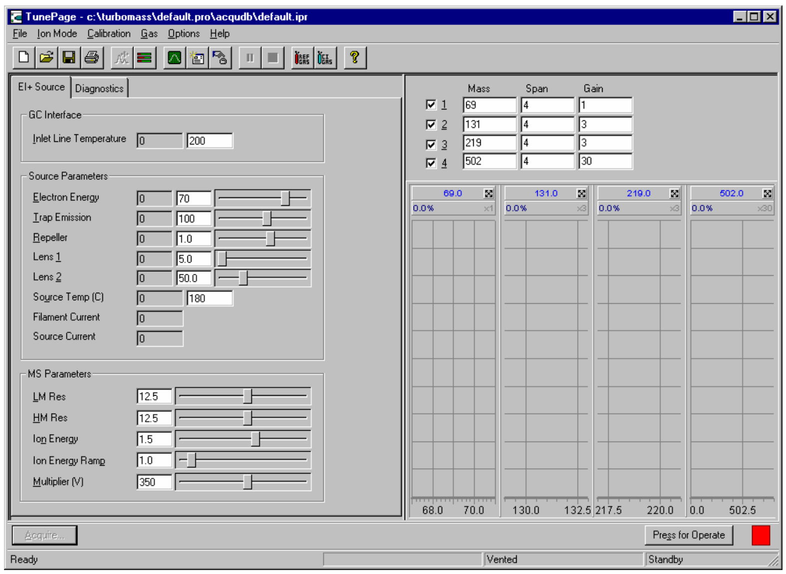
Select **Diagnostics Page** (a checkmark appears in the menu) in the Tune **Options** menu to display diagnostic information. This information includes turbomolecular pump speed, voltages to vacuum gauges, reference voltages (+5 and 0 volts), and the prefilter bias reference voltage.

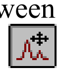
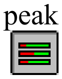
Instrument Tuning 5

The Tune Page

Before acquiring data, you may need to check the tuning conditions of the instrument, and if necessary, modify one or more of the instrument tuning parameters. The instrument can be tuned either manually or automatically from the instrument Tune page.

The Tune page is a configurable paneled display. Use the **Ion Mode** menu to display parameters for EI+ (electron ionization), CI+ (positive chemical ionization), or CI- (negative chemical ionization), depending on your ionization source. The left side of the window contains the mass spectrometer tuning parameters.



The panel in the top right of the window can display either the tune peak information or instrument pressure information. The display can be switched between tune peak information and instrument vacuum pressure information using the  and  toolbar buttons.

A toolbar displayed at the top of the Tune page allows you to perform some common operations with a single click of the appropriate toolbar button.

At the bottom right of the window is the Tune peak display. You can display up to four masses to tune on. The number of tune peaks displayed is controlled by the four checkboxes in the top right panel. Any one of the tune peaks can be zoomed so that it occupies the entire tune peak area. When a tune peak has been zoomed, the controls for the mass and span for that peak are displayed at the top of the display window.

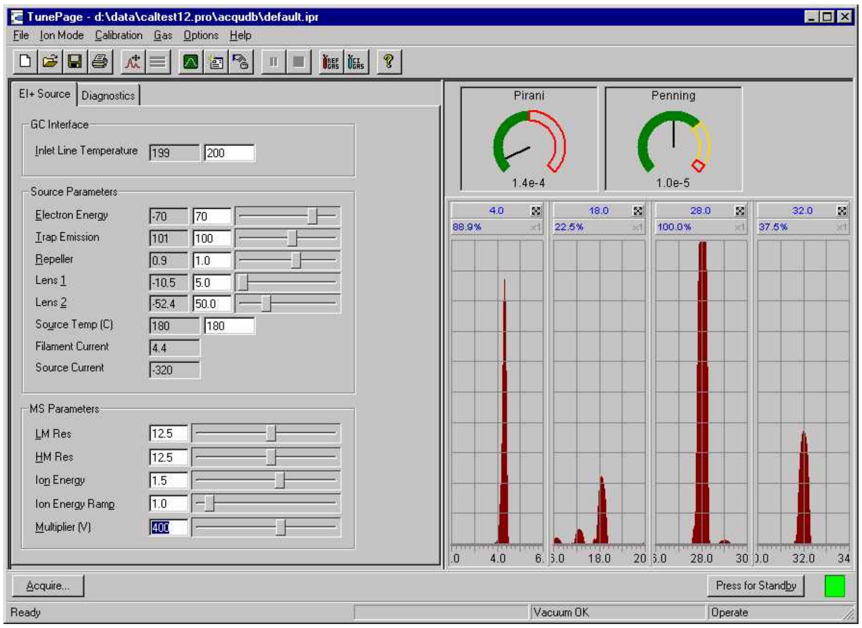


Figure 6 Tune Page showing instrument pressure information

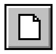
Displaying the Tune Page

1. Click  in the MS portion of the instrument status panel in the TurboMass top level window.

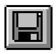
2. From the Tune **Options** menu, select either **Peak Editor** to show peak information, or **Vacuum Monitor** to show instrument vacuum pressure information.

The Tune Page Toolbar

The toolbar is displayed at the top of the Tune page and allows you to perform some common operations with a single click of the appropriate Toolbar button.

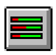
 Loads the default file.

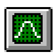
 Selects a data file.

 Saves current Tune parameters to disk.

 Prints current window in portrait format.

 Displays Tune peak information.

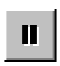
 Displays instrument vacuum pressure information.

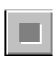
 Edits scope settings.

 Resets the zero level of the instrument and reinitialize the system.

 Activates Standard UltraTune (DFTPP/BFB Tune)

 Activates Custom UltraTune (AutoTune)

 Pauses an acquisition. Toggles to continue the acquisition. This does not affect the acquisition of data from samples being processed in the Sample List.

 Stops an acquisition.

Toggles CI gas on/off.

Toggles reference gas on/off.

 Accesses online Help.

Changing Tune Parameter Settings

Most of the tuning parameters can be set using the slider bar or by editing a text field. The tuning parameters can be modified in any of the following ways:

- by dragging the slider bar using the mouse;
- by entering a new value directly into the text field;
- by pressing the left or right keyboard arrows after clicking on the slider bar.

If you change a tune parameter using the slider bar, the value shown in the text field will update as appropriate.

Other tune parameters only have a text field and can only be changed by direct typing.

The speed with which the system will respond to changes in parameter settings is controlled by the speed with which the peak display refreshes. To get the sliders to be most responsive you should lower the scope scan speed and inter scan time (for more information, see *Setting Scope Parameters* on page 103.)

Printing Tune Information

A report of the tuning parameters can be sent to the printer by clicking  or by selecting **Print** from the Tune **File** menu. This report contains a copy of the tune peak information displayed on the screen, along with a record of each parameter setting.

You can also automatically print out a Tune report by selecting the Print Report Target Tune option. See *UltraTune* on page 93.

Experimental Record

Tuning parameters are stored with every data file as part of the experimental record. The tuning parameters for a particular data file can be viewed or printed from the Data Browser.

Saving and Restoring Parameters

Whole sets of instrument tuning parameters can be saved to disk as a named file and then recalled at a future date.

NOTE: *A tune parameter file contains the latest settings for the source parameters for* ***all*** *supported ionization modes, not just the ionization mode you are currently using. Tune parameter files also contain settings for the analyzer, and GC inlet line (transfer line) temperature setpoint.*

Saving a Set of Parameters

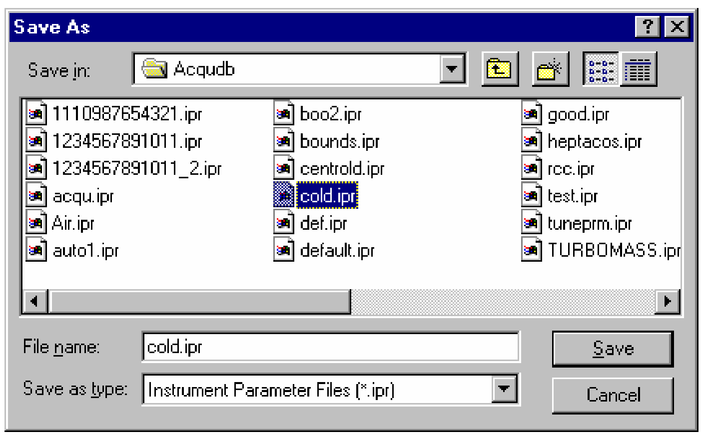
1. To save the current tune parameters with the existing file name, click 

   OR

   Select **Save** from the Tune **File** menu.

   To save the current tune parameters with a new file name, select **Save As** from the Tune **File** menu.

2. Enter a new file name under which you want the parameters to be saved, or alternatively select an existing file from the list displayed.



3. Click **Save**.

   If the selected file already exists on disk, you will be asked to confirm that you want to overwrite the existing information. Click **Yes** to continue or **No** to enter a different file name.

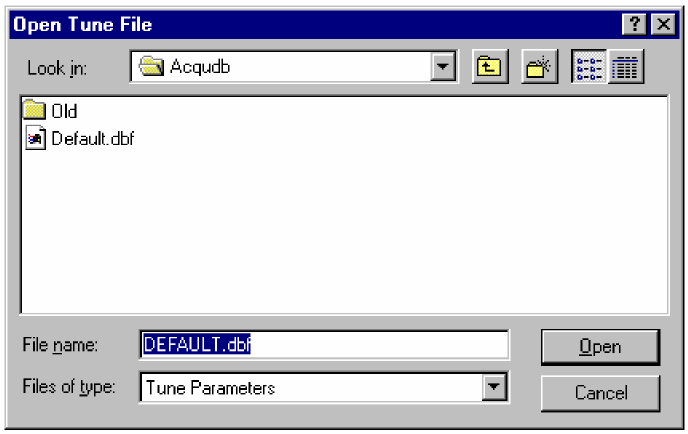
NOTE: *If you close the Tune page without saving any new settings, the software will prompt you to save the file.*

Restoring a Saved Set of Parameters

1. Click 

   OR

   Select **Open** from the Tune **File** menu.

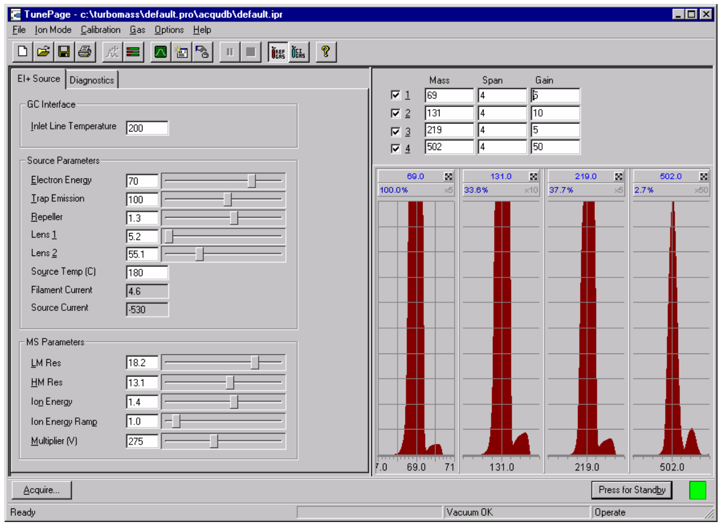


2. Select the tuning parameter set that you want to use, either by entering its name or by selecting it from the displayed list.

3. Click **Open** to open the Tune File dialog.

Modifying the Peak Display

The Tune peak display is modified using either the tune peak parameters, or by using the mouse directly on the Tune Peak display.



Selecting Peaks

1. Select the number of peaks that you want to display by selecting the appropriate checkboxes in the top right panel of the Tune page.

   For example, if you want to display only the first and second tune peaks, then select checkboxes 1 and 2, and deselect checkboxes 3 and 4.

2. Click 

   OR

   Select **Peak Editor** from the Tune **Window** menu. Then, for each active peak, select the mass that you want to tune on, the span, and the gain.

Zooming or Unzooming a Peak

Drag the mouse horizontally or vertically to define a larger area. The peak is expanded to fill this area.

OR

Click  to return the peak to the original size.

To Change the Tune Mass, Span or Gain

- Edit the mass, span or gain in the text fields above the peak display.

- Double-clicking on the borders above or below the peak will increase or decrease the peak intensity by a factor of 2.

NOTE: The span specifies a small mass window applied centrally about the highlighted mass. When specifying a mass that is close to either the low mass limit (1) or high mass limit (1205), you must first enter a span that does not force the mass outside of the mass limits. For example, to specify a mass of 2, you must first enter a span of 2 or less.

UltraTune

TurboMass can automatically tune the mass spectrometer by using UltraTune with an EI ion source. UltraTune ramps the settings for the tuning parameters until they are optimized to give good intensity, resolution, and peak shape.

Reference Gas and Filament Control

Since reference gas is always required for the UltraTune process, the TurboMass software will assume control for switching the flow on and off.

Tune History

A 'tune history' file is maintained that records the tune parameters following a successful UltraTune. It is saved in an ASCII, comma–separated format, with one tune record per line. The file is located in the main 'TurboMass' directory. Each new successful UltraTune will append a new line to the end of the file.

If the tune history file does not exist when a record comes to be written to it, it will be created. The first line of the file will contain names for each field in the record, which may be used as column headings when the data are imported into Excel. The tune history file is named "UltraTuneHistory.CSV" and it is located in the primary TurboMass path (C:\TurboMass\).

NOTE: *The goal of Standard UltraTune is to give a satisfactory, library-searchable spectrum, not to achieve maximum sensitivity.*

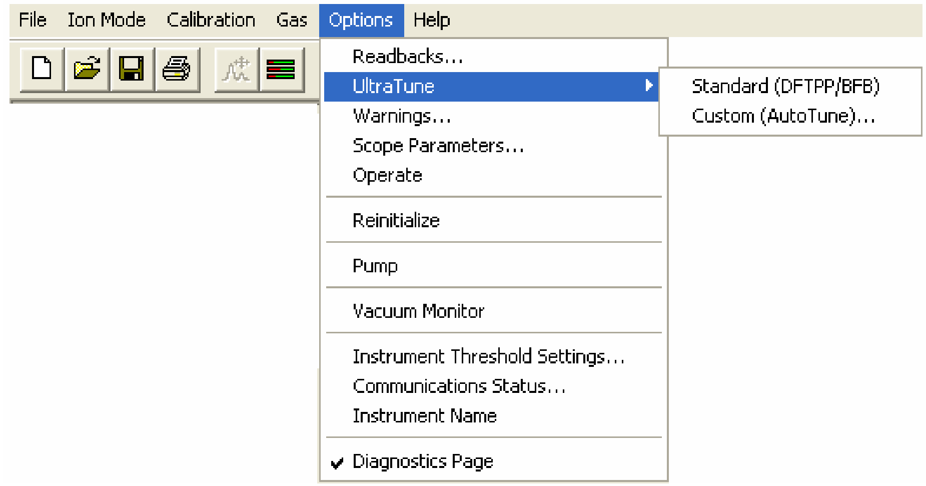
Running Standard UltraTune (DFTPP/BFB)

NOTE: *If you cancel UltraTune during the data acquisition phase, the instrument will be restored to the state it was in prior to the start of UltraTune (i.e., previous tune parameters, reference gas off, etc).*

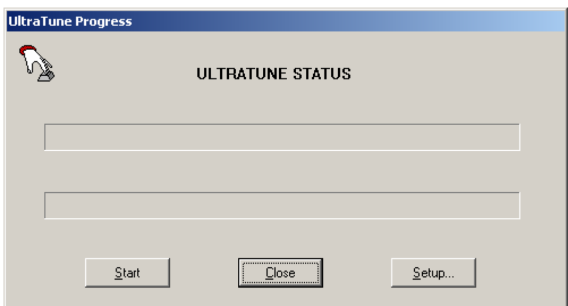
1. Click 

   OR

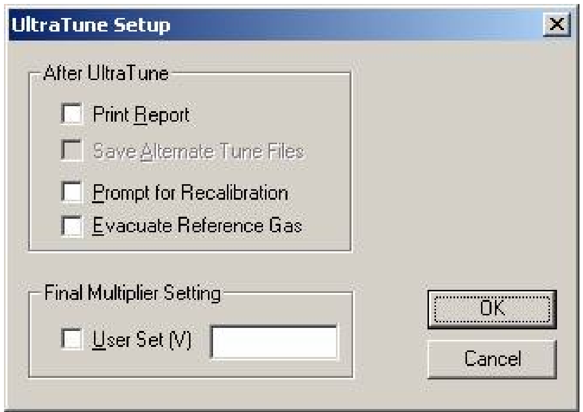
Select **UltraTune**, followed by **Standard (DFTPP/BFB)** from the Tune page **Options** menu.



You will hear a click when the reference gas solenoid valve opens and *UltraTune* begins. The first page of *UltraTune* is displayed.



2. Click **Setup** to display the *UltraTune Setup* dialog.



The default setup parameters (Full Width Half Max **(FWHM)** = 0.55 for masses 69, 131, 219, and 502) for EI UltraTune are suitable for tuning with Heptacosa. There is no need to alter the Tune Mass or Peak Width parameters if you are using Heptacosa.

The Full Width at Half Max parameters set the peak width at half height for the Low and High Masses being monitored. Typical values are 0.55 for both, but applications requiring higher mass resolution (e.g., the environmental BFB tune) or more accurate isotope ratios may need higher resolution (e.g., 0.50) with Custom UltraTune.

3. Select your **After UltraTune** settings:

   Print Report - Automatically prints a tune report after a successful UltraTune.

   Save Alternate Tune Files - Saves the top three UltraTune result sets as tune files rather than just the top one.

   Prompt for Recalibration - Prompts you to perform a mass calibration after a successful UltraTune.

   Evacuate Reference Gas - Automatically pumps out the reference gas following UltraTune

4. Set the Final Multiplier Setting.

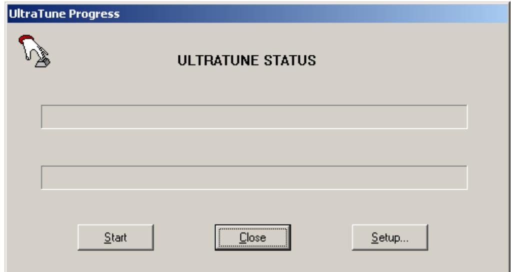
User Set (V) - Check this box if following UltraTune, you want to set the PMT voltage to the value you enter in the field.

5. When you are satisfied with the **UltraTune Setup** parameters, choose **OK** to exit this dialog.

6. Choose **Start** to start UltraTune and the following occurs:
   - If the source is not at the set temperature (within normal tolerance) then the message "Waiting for the source temperature to equilibrate" is displayed in the UltraTune Status dialog.
   - Once the source reaches the set temperature, if Operate is Off, Reference Gas is Off or Pump Out Reference Gas in On, the message "Waiting for Reference Gas pressure to stabilize" will be displayed.
   - If Pump Out Reference Gas is On it will be turned off, followed by a delay of 50 seconds.
   - If Reference Gas is Off it will be turned on, followed by a delay of 100 seconds. The "Waiting for Reference Gas pressure to stabilize" message will then be removed.
   - If Operate is Off it will be turned on, followed by a delay of 5 seconds. A check is then made to determine if the Electron Energy and Trap Emission current are at the set values (within ±7 and ±10 respectively). If either (or both) readbacks are out of tolerance the error message is displayed is "Electron energy not at the set value." And/or "Trap emission current not at the set value" and the UltraTune procedure stopped.

The *UltraTune status* dialog is displayed.

The status dialog displays the part of the tuning process that is currently occurring. The UltraTune status bar is updated to show the progress of UltraTune.



7. When *UltraTune* has finished, the UltraTune completed message is displayed.

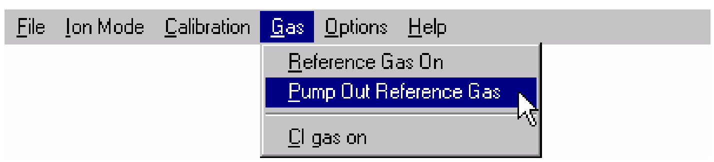
   Click **OK**.

   The tuning parameters determined by *UltraTune* will be saved to the *current tune parameter file*.

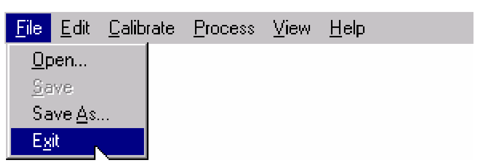
If the *Prompt for Recalibration* box was checked in the *UltraTune Setup* dialog, you will begin to mass calibrate. Refer to Chapter 6, Mass calibration for details.

If you selected Evacuate reference Gas in the UltraTune Setup dialog, UltraTune turns off the Reference Gas and the pumps out the reference gas.

NOTE: You can verify if it has been done by selecting **Reference Gas On** from the *Gas* menu to remove the check mark (✓) and selecting **Pump Out Reference Gas** from the *Gas* menu and wait about one minute as the reference gas is pumped away. Select **Pump Out Reference Gas** from the *Gas* menu again to remove the check mark and stop pumping the gas.



8. Select **Exit** from the *File* menu.



Running UltraTune Custom (AutoTune)

TurboMass can automatically tune the mass spectrometer using UltraTune Custom with an EI ion source. UltraTune Custom ramps the settings for the tuning parameters until they are optimized to give good intensity, resolution, and peak shape.

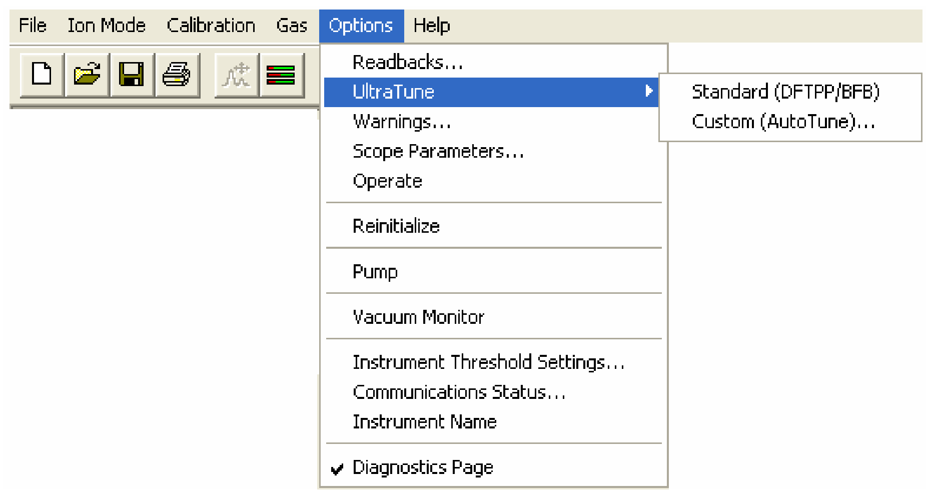
NOTE: *The goal of UltraTune Custom is to give a satisfactory, library-searchable spectrum, not to achieve maximum sensitivity.*

Running UltraTune Custom

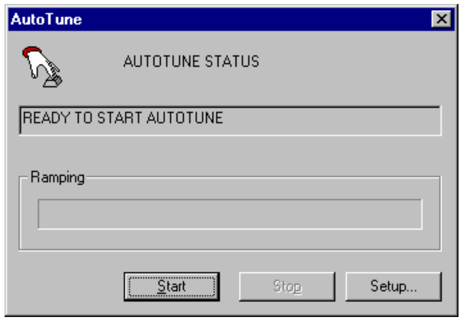
1. Click 

   OR

   Select **UltraTune**, followed by **Custom (AutoTune)** from the Tune page **Options** menu.



NOTE: *The instrument must be in Operate mode and the reference gas must be on before you can run UltraTune Custom (AutoTune).*



2. Click **Setup** to set the AutoTune setup parameters.

   The default setup parameters (FWHM = 0.6 and masses 69 and 502) for EI UltraTune are suitable for tuning with Heptacosa. There is no need to alter the **Tune Mass** or **Peak Width** parameters if you are using Heptacosa.

   The Level of AutoTune performed can be selected as **Maintenance** or **Full**.

   A **Full** AutoTune starts from a default set of tuning parameters, but uses your current settings for the **Inlet Line Temperature** and **Source Temperature**.

   In a Maintenance AutoTune, the software uses your current settings for Inlet Line Temperature, Source Temperature, Electron Energy and Source Emission.

   A **Maintenance** AutoTune can be quicker than a **Full** AutoTune, but should only be performed if the instrument is reasonably well tuned already. If the current tuning is too poor, AutoTune will give an error and ask you to perform a **Full** AutoTune.

   The Tune Masses parameters set a **Low Mass** and **High Mass** that will be used to tune on.

   The **Peak Width at Half Height** parameters set the peak width at half height for the **Low** and **High Mass**es being monitored. Typical values are 0.6 for both, but applications requiring higher mass resolution (for example, the environmental BFB tune) or more accurate isotope ratios may need higher resolution (for example, 0.55 or 0.50).

   SIR sensitivity may be improved by selecting a number larger that 0.6, but care must be taken to avoid nearby eluting peaks with ions one m/z above or below the target ion.

3. Click **OK**.
4. When you are satisfied with the AutoTune setup parameters, click **OK** to exit.
5. Click **Start** to start AutoTune.

   TheAutoTune status bar is updated to show the progress of AutoTune. AutoTune has seven stages. The AutoTune stages are listed here.

1	**Checking instrument conditions**	AutoTune checks that Tune page readbacks are within acceptable tolerance.
2	**Attempting to detect initial beam**	AutoTune looks for an initial beam by increasing the value of the multiplier.
3	**Rough tuning focus lenses at low mass**	Values of lenses are ramped to see where the low mass peak intensity maximizes.
4	**Tuning ion energy and ion repeller**	Ramps values for ion energy ramp, ion energy and repeller for best sensitivity consistent with lowest values for these parameters.
5	**Tuning for good peak shape**	Checks peak width at half height and height of valley between main and isotope peaks.
6	**Fine tuning focus lenses at high mass**	Values of lenses are ramped over a narrower range using the values determined in stage 4 to see where the high mass peak intensity maximizes.
7	**Tuning multiplier for good sensitivity**	The value of multiplier ramped until the low mass peak intensity is 80 % of full scale.

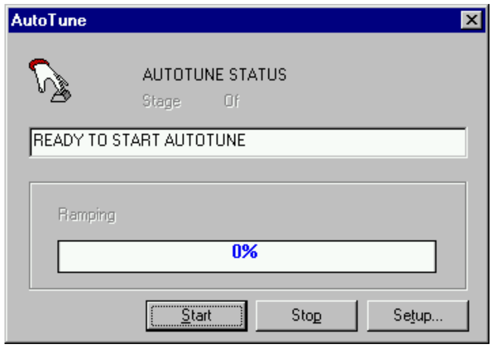
   When AutoTune has finished, it displays a status message indicating that AutoTune has been successfully completed.

1. Click **OK** to return to the Tune page.

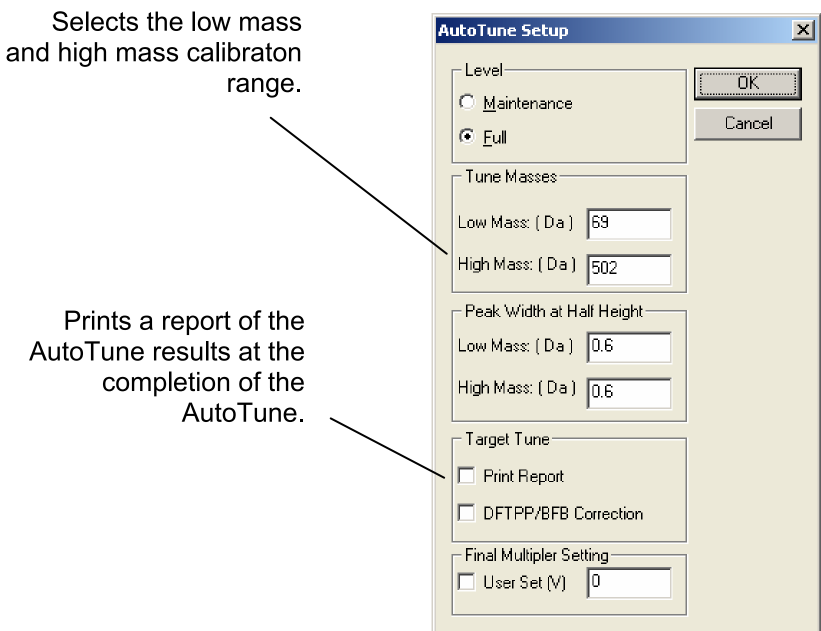
   The tuning parameters determined by AutoTune will be saved to the current tune parameter file.

2. Click  to start *AutoTune*.

   You will hear a click when the reference gas solenoid valve opens and *AutoTune* begins. The first page of *AutoTune* is displayed.

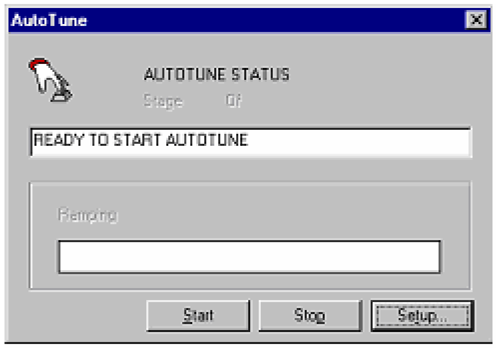


3. Alternatively, you can click **Setup** to display the *AutoTune Setup* dialog and customize your Tune parameters.



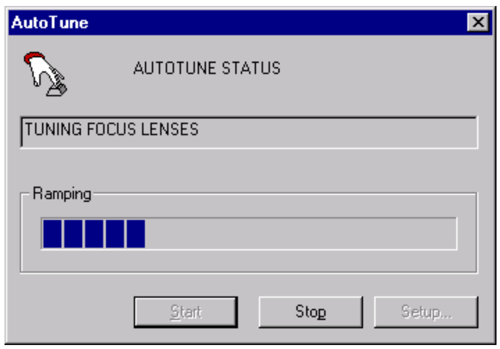
4. Click **OK** to accept the *setup parameters*.

   The *AutoTune* dialog appears with the message *Ready To Start Autotune*.



5. Click **Start** to start AutoTuning the mass spectrometer.

   The *AutoTune status* dialog is displayed.

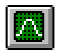


The status dialog displays the part of the tuning process that is currently occurring. The AutoTune status bar is updated to show the progress of AutoTune. AutoTune has seven stages.

Setting Scope Parameters

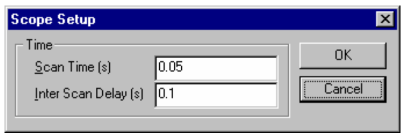
Various parameters can be set to control the peak display. You can control the speed at which the display is refreshed.

Changing the Scope Setup

1. Click 

   OR

   Select **Scope Parameters** from the Tune **Options** menu.

2. Make any required changes to the settings.

3. Click **OK**.

Scan Time and Inter Scan Time Controls the speed with which the Tune peak display is updated. The tuning system will behave more responsively if the scan time and inter scan time are short.

The following options are available by right-clicking on the spectrum plot on the Tune page.

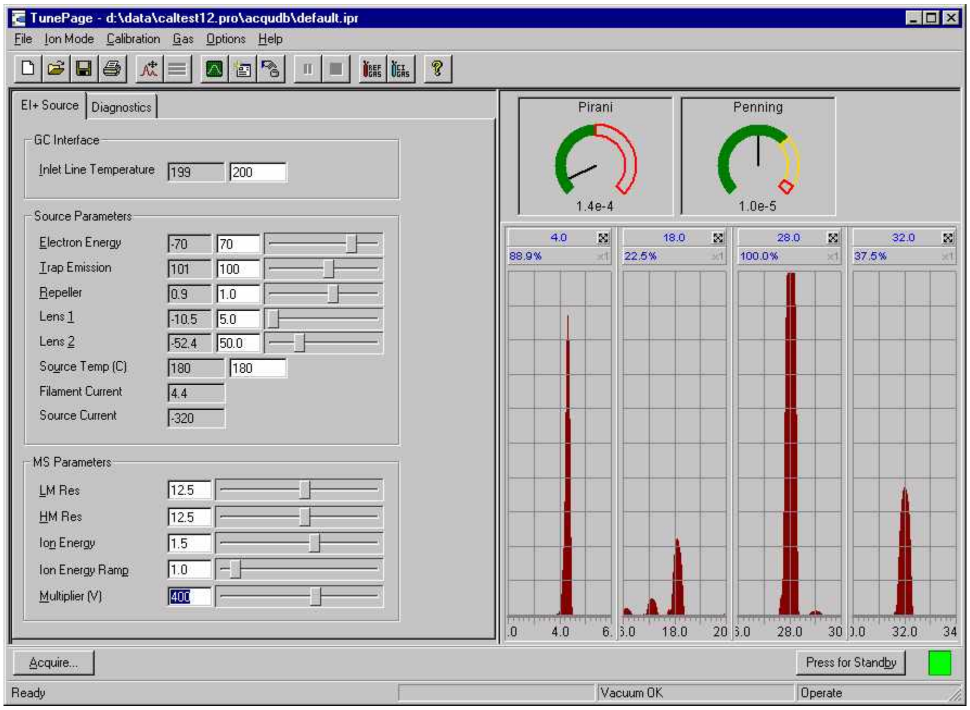
Grid Select **Horizontal and/or Vertical** (a check mark appears in the menu) to display a horizontal grid and/or vertical grid on the peak display.

Intensity When this parameter is set to **Relative Intensity**, the percentage intensity of the base peak in the active tune segment window is displayed. When this parameter is set to **Absolute Intensity** the absolute intensity of the base peak in the active tune segment window is displayed. When this parameter is set to **Normalize**, all peaks are rescaled relative to the largest peak.

Changing Inlet Heaters

The GC Interface Inlet Line Temperature setting on the Tune page is used to set the temperature of the interface between the gas chromatograph and the mass spectrometer.

Enter the desired temperature (ºC) in the text field.



Setting Gas Controls

The **Gas** menu on the Tune page lets you turn gasses on or off.

Turning a Gas On or Off

- Click the appropriate toolbar button

  OR

  Select the required gas from the Tune **Gas** menu.

  If the gas was previously turned off, it will now be turned on. A check mark will appear next to a gas if it is turned on.

Pump out Reference gas should be used for about one minute prior to the first time Reference gas is selected, to remove the air from the vial. It should also be used whenever the vial is refilled.

Vacuum

The mass spectrometer's vacuum system can be controlled from the Tune page. Be sure that this is done in accordance with the information in your *Mass Spectrometry Hardware Guide.*

Pumping Down the Vacuum System

1. Select **Pump** from the Tune **Options** menu.

   The menu name will change from **Pump** to **Vent**, and the system will begin its pump-down sequence.

2. To monitor the vacuum progress with the optional vacuum gauges, select **Vacuum Monitor** from the Tune **Options** menu.

Venting the Vacuum System

Select **Vent** from the Tune **Options** menu, and confirm that you want to vent the system.

The system will start its automatic venting sequence.

Warning Messages in Tune

Select **Warnings** from the Tune **Options** menu to display a dialog containing a list of optional warning messages. In most cases, these warnings should all be selected.

You can select the following warning messages when exiting Tune under the following conditions:

- The filament on.
- The reference gas on.
- The Pump out reference gas on.
- The CI gas on.

You can select the following warning messages when venting the mass spectrometer with:

- a hot ion source (> 100 °C);
- a hot GC transfer line (> 100 °C).

Resetting the Zero Level

The **Reinitialize** command measures the position of the noise signal so that any baseline offset caused by the electronics or instrumentation can be compensated for. It is advisable to reset the zero level whenever the value of the multiplier voltage is changed.

- You can reposition the zero level (or Baseline) by clicking 

  OR

  Select **Reinitialize** from the Tune **Options** menu.

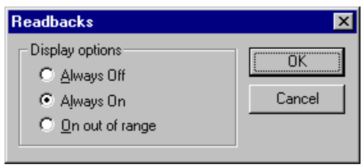
Controlling Readbacks

TurboMass allows you to choose how system readbacks will be displayed on the Tune page. You can ask for readbacks to be displayed continuously, never, or only when they differ from their associated set points by more than 10 %.

Note that a number of the readbacks are for diagnostic purposes only and thus do not need to be very precise. Their function is to indicate if the voltage is present or not. The acceptable variation between the set value and the readback value will vary depending on the particular tune parameter. If you are concerned about the values, contact your local service office for advice.

Changing Readback Style

1. Select **Readbacks** from the Tune **Options** menu.



2. Select the readback style required.

   Selecting **Always On** will always display readbacks. Selecting **Out of Range** will display readbacks when they differ from their associated set points by more than 10 %.

3. Click **OK**.

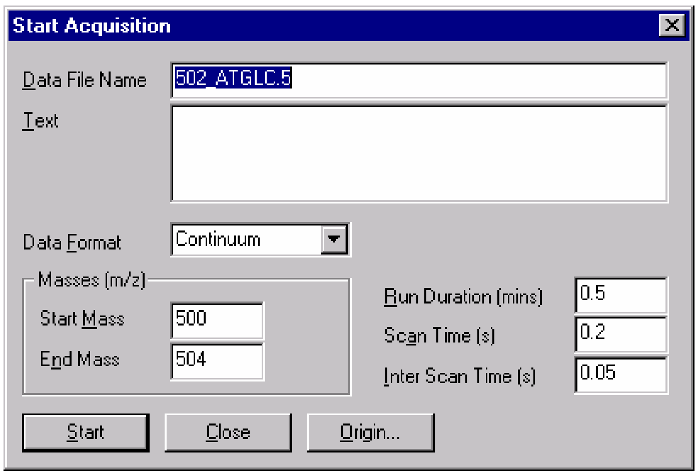
Starting an Acquisition from the Tune Page

The easiest way to acquire data for a sample is to acquire it directly from the Tune page. You cannot use inlet programs (for example, GC methods) from the Tune page, acquire analog data or acquire multiple sample sequences, but you can start and stop acquisitions and control most of the scanning parameters.

1. Select **Acquire** from the Tune **Window** menu

   OR

   Click **Acquire** at the bottom of the Tune page.



2. Make any required changes to the settings.

Data File Name — The name of the data file to which acquired data will be written. The filename can be up to 128 characters. If the file exists, you will be asked if you want to overwrite it.

Text — A text area that is used to enter the sample description. The description can be displayed on any output of the acquired data and has a maximum length of 80 characters.

Data Format	The type of data that will be collected and stored on disk. It can be Centroid, Continuum or MCA.
Start Mass	Specifies the mass at which the scan will start. The **Start Mass** must be lower than the **End Mass**.
End Mass	Specifies the mass at which the scan will stop.
Run Duration	Length of the acquisition, measured in minutes.
Scan Time	Specifies the duration of each scan in seconds.
Inter Scan Time	Specifies the time in seconds between a scan finishing and the next one starting. During this period data is stored on the PC.

3. Click Start Acquisition.

Mass Calibration 6

Introduction

TurboMass provides a fully automated facility for calibrating the mass scale of an instrument.

To open the main calibration dialog, select **Calibrate Instrument** from the **Calibration** menu on the Tune page.

How A Calibration Is Formed

A mass spectrum of a reference compound (a calibration file) is acquired and matched against a table of the expected masses of the peaks in the reference compound that are stored as a reference file. Each peak in the reference file is matched to a corresponding peak in the calibration file. The mass differences between the reference peaks and calibration peaks are the calibration points. A calibration curve is fitted through the calibration points.

The vertical distance of each calibration point from the curve is calculated. This distance represents the remaining (or residual) mass difference after calibration.

The standard deviation of the residuals is also calculated. This number is the best single indication of the accuracy of the calibration.

Calibration Types

TurboMass requires up to three calibration curves:

- A static calibration is used to accurately 'park' the quadrupole mass analyzer on a specific mass of interest (in Tuning and SIR, for example).

- A scanning calibration enables peaks acquired in a scanning acquisition to be mass measured accurately.

- A scan speed compensation calibration compensates for 'lag time' in the system when the instrument is scanned rapidly.

A separate mass spectrum of the reference compound is acquired for each selected calibration type.

Overview Of The Calibration Process

Check the Instrument Tuning

The mass spectrometer should be in Operate mode with Reference gas on. Check that the peak shape and intensities are correct.

Set the Calibration Parameters

1. Select the appropriate reference file for the calibration reference sample that you are going to use (typically HEPTA.REF).

2. If required, set the automatic calibration checking parameters in the AutoCal Check Parameters dialog.

   These parameters control how closely the recorded data must match the reference file.

3. If required, set the **Peak Match** and **Curve Fit** parameters in the Calibration Parameters dialog.

   These parameters control the location of reference peaks in a calibration spectrum, and the drawing of a calibration curve to correct the resulting mass differences.

4. If you are calibrating continuum or MCA data types you should set the **Mass Measure** parameters.

   These parameters control peak detection in continuum and MCA data. There is no need to set these parameters if you are using centroided acquisition, the typical GC/MS data acquisition mode.

Start an Automatic Calibration

1. From the main Calibrate dialog, click **Calibrate/Start Acquisition** to open the Automatic Calibration dialog.

2. Select the types of calibration you want to perform.

Usually, all checkboxes should be selected.

3. Select **Acquire & Calibrate** to perform automatic calibration.

4. Optionally, select **Acquire & Verify**.

5. Select **Print Report** if you want a printed calibration report.

6. Set the data **Acquisition Parameters** if your mass range or data acquisition rates are not covered by the defaults.

7. Click **OK**.

Check the Calibration Report

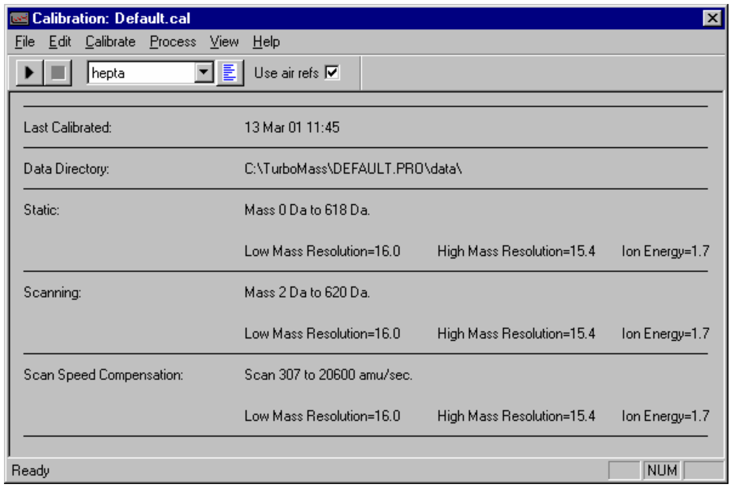
Examine the calibration report and display the calibration graphs, if necessary, to satisfy yourself that the calibration is satisfactory.

A good calibration will cover your data acquisition mass range and have a small (typically less than ± 0.3) error for each calibration mass.

Displaying Calibration Parameters

The Calibration dialog displays calibration status information, including calibrated mass range and scan speeds, and the time and date of the last calibration.

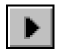
1. To open the Calibration dialog, select **Calibrate Instrument** from the **Calibration** menu on the Tune page.

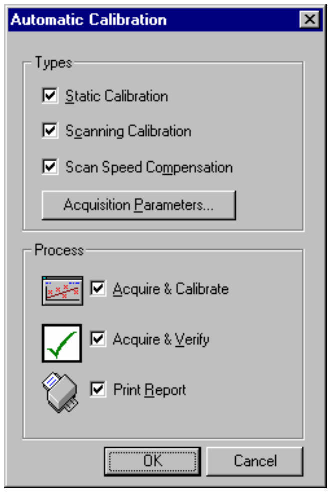


Setting Parameters that Control Calibration

Use the following procedures to set calibration parameters.

Setting Automatic Calibration Parameters

1. Click  in the Calibration dialog to open the Automatic Calibration dialog.



2. Select Static Calibration, Scanning Calibration, or Scan Speed Compensation, as appropriate.

   Usually all checkboxes should be selected.

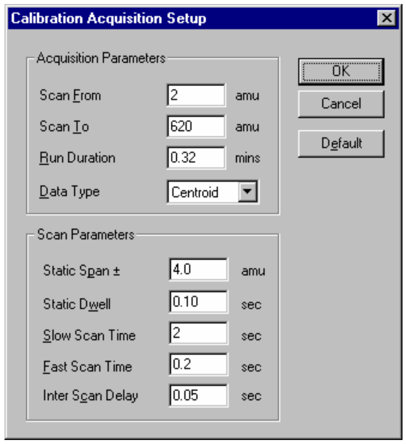
3. Optionally, select **Acquire & Verify** to acquire a calibrated mass spectrum of the reference compound.

4. To automatically print a report of the calibration when the calibration is complete, select **Print Report**.

   If you choose not to print the report at this stage, you can always print it from the calibration curve display later. The report contains pictures of the calibration curves produced, along with calibration statistics such as standard deviation.

Setting Data Acquisition Parameters

1. Click **Acquisition Parameters** in the Automatic Calibration dialog to open the Calibration Acquisition Setup dialog.



2. Specify the acquisition parameters.

Scan From and **Scan To**	Specify the scan range for each calibration type.
Run Duration	Specifies the data acquisition time for each calibration data file. It is usually calculated by the software.
Data Type	Specifies whether data will be acquired in centroid, continuum or MCA mode. It is recommended that the calibration uses the same data type as the sample data you will be acquiring. GC/MS uses the Centroid type almost exclusively.

3. To acquire data for static calibration, the portion of the mass scale immediately around each reference peak is scanned.

Static Span	Specifies the distance to be scanned either side of the reference peak. Typically set to 4.

Static Dwell Specifies the time taken to scan the static span range. Typically set to 0.1.

4. To acquire data for scanning calibration, the mass scale is scanned over the selected range, in a time specified by the **Slow Scan Time** parameter. This should be as long or longer than the slowest rate you will use. Typically set to 2.

5. To acquire data for the Scan Speed compensation calibration, the mass scale is also scanned over the selected range, in a time specified by the **Fast Scan Time** parameter. This should be as fast or faster than the fastest scan rate you will use. Typically set to 0.1.

   Inter Scan Delay specifies the time between one scan ending and the next scan starting. If this is too short (typically less than 0.05 sec), the recorded spectra may be incomplete depending upon mass range. Typically set to 0.1.

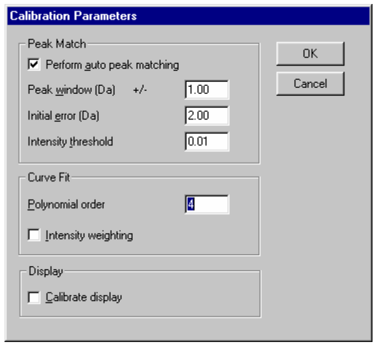
   Very fast scanning over wide mass ranges may require verifying that all data are properly written to the data file. The mass calibration should also be carefully checked.

6. To reset all parameters to their default values, click **Default**.

Setting Calibration Parameters

1. Select **Calibrate Instrument** from the Tune **Calibration** menu to open the Calibration dialog.

2. Select **Calibration Parameters** from the Calibration **Edit** menu to open the Calibration Parameters dialog.



3. Specify the **Peak Match**, **Curve Fit**, and **Display** calibration parameters.

Perform auto peak matching Select this to turn on auto peak matching. When unselected, automatic peak matching is turned off.

Peak window Specifies the maximum mass difference between the remaining reference peaks and the *expected* position of the corresponding peaks in the acquired spectrum. Normal operating range for the Peak Window parameter is 0.3 to 1.5 Da. It may need to be large (for example, 4) for very high mass work.

Initial error The first reference peak to be matched is chosen to be close to the center of the calibration mass range. The **Initial error** parameter specifies the maximum mass difference between this reference peak and the corresponding peak in the acquired spectrum. Normal operating range for the **Initial error** parameter is 0.5 to 2.0 Da.

Intensity threshold Any peak in the acquired spectrum with intensity less than the specified **Intensity threshold** will not be used to form the calibration curve. The threshold is specified as a percentage of the most intense peak in the acquired spectrum. Normal operating range for the **Intensity threshold** parameter is 0 to 5 %.

Polynomial order When each peak in the reference spectrum has been matched with a corresponding peak in the acquired spectrum, the mass difference

acquired mass - reference mass

is calculated for each pair of peaks. These mass differences are plotted as points on a graph. Each data point has the mass of the acquired peak as its x coordinate and the above mass difference as its y coordinate. A smooth curve is drawn through the points. The **Polynomial order** parameter controls the type of curve that is drawn and can be set to any value between 1 and 5. If Polynomial order = 1, a straight line is drawn through the points. If Polynomial order = 2, a quadratic curve is drawn through the points. If Polynomial order = 3, a cubic curve is used.

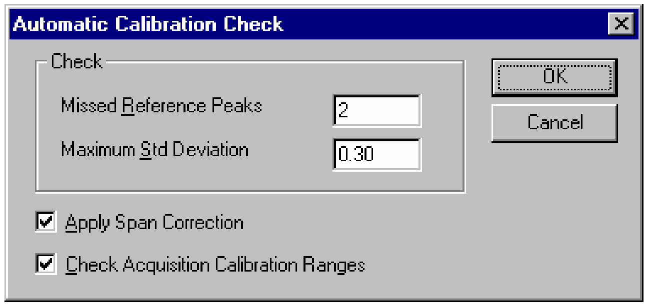
For a typical EI calibration where the mass range calibrated starts below 100 amu and extends up to 650 amu, the recommended setting for the Polynomial order parameter is 4.

Intensity weighting If selected, the curve fit is weighted toward the points representing the more intense acquired peaks. The weight of each point is proportional to the square root of the intensity of the acquired peak.

Calibrate display If selected, enables calibration of the peaks in the top (raw file) graph. This feature allows selection of one peak at a time, with the display being recalibrated after the selection of each peak, bringing the other masses in the spectrum into line.

Setting Automatic Calibration Check Parameters

1. Select **AutoCal Check Parameters** from the Calibration **Edit** menu to open the Automatic Calibration Check dialog.



2. Specify the AutoCal Check parameters, and click **OK**.

Missed Reference Peaks Allows you to enter a number of consecutive peaks from the reference file that the system is allowed to miss before a warning is issued to the user.

Maximum Std Deviation Performs the same function as **Missed Reference Peaks** if the residuals for a particular calibration exceed the number entered.

Apply Span Correction Applies an extra correction to the mass scale that is dependent on the mass range being scanned. This correction ensures that mass assignment will be correct even if the mass scale that you are working with is different from the one that the instrument was originally calibrated over. It is not recommended that this option be used if the mass range of interest is less than 1000 amu and includes the range 0 - 150 amu.

Check Acquisition Calibration Ranges If selected, a message is displayed if an acquisition is started that is outside the range of the current calibration.

Setting Mass Measures

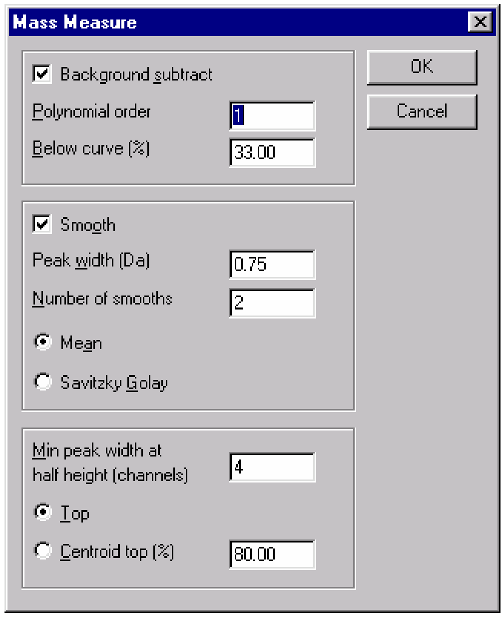
If you are using continuum or MCA acquisition modes to acquire your calibration data, you will need to tell the system how it should convert the acquired data into

centroided data needed by the calibration process. For more information on Mass Measure parameters, see *Spectrum* on page 423.

Setting the Mass Measure Parameters

1. Select **Mass Measure Parameters** from the Calibration **Edit** menu to open the Mass Measure dialog.

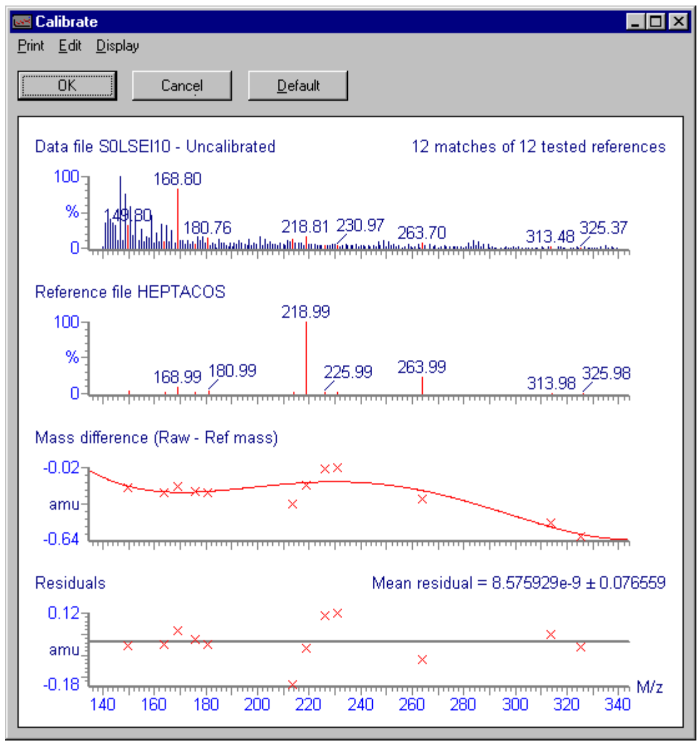
2. Enter the required parameters and click **OK**.



The Calibration Report

The peak matching algorithm performed by the calibration may have found wrong peaks, or missed some peaks. You may need to change the peak match parameters or adjust the peak matching manually. You can change the peak match parameters by selecting **Peak Match Params** from the calibration graph **Edit** menu. If the peak matching algorithm has found the wrong peaks, increasing the value of the **Peak window** parameter will solve the problem. You should also try reducing the value of the **Intensity threshold** parameter (if it is not already zero), before identifying the peaks in the acquired spectrum by hand.

The top graph shows the calibration spectrum. The peaks matched to reference peaks are highlighted in a different color.



Altering the Displayed Range

You can alter the range of the spectrum on display by left-clicking at one end of the range of interest, and dragging the mouse to the other end of the range of interest.

TurboMass indicates the selected range. Clicking **Default** restores the default display range.

Manually Matching Peaks

- You can match a calibration peak to the closest reference peak by positioning the mouse over the calibration peak in the top window, and right-clicking.

  If the closest reference peak is already matched to another calibration peak, the previous match will be removed.

- You can also right-click to undo a peak match. Position the mouse over the matched calibration peak and right-click.

  For small peaks, this must be done very close to the baseline.

Other Calibration Facilities

Deleting the Instrument Calibration

1. Select **Delete Calibration** from the Calibration **Calibrate** menu.
   This restores the instrument to an uncalibrated state.

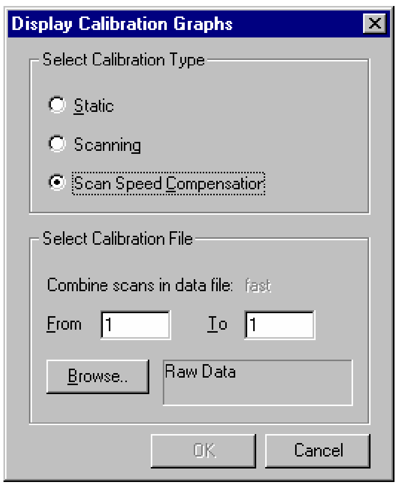
2. In the confirmation dialog, click **OK** to delete all instrument calibration

   OR

   Click **Cancel** to abort the operation.

Displaying a Calibration Graph

1. Select **From File** from the Calibration **Calibrate** menu to open the Display Calibration Graphs dialog.



2. Select the desired Calibration Type: **Static**, **Scanning**, or **Scan Speed Compensation**.

3. Click **OK**.

Displaying a Verification Graph

You can display the verification graphs for a particular calibration type. Normally an acquisition would be performed and a calibration made. Use this process to reprocess the data using the calibration file to verify the accuracy of the calibration.

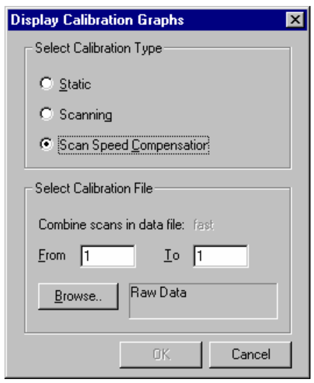
1. Select **Verification From File** from the Calibration **Process** menu to open the Display Verification Graphs dialog.

2. Select the desired Calibration Type: **Static**, **Scanning**, or **Scan Speed Compensated**.

3. Click **OK**.

Making a Calibration from a Data File

1. Select **From File** from the Calibration **Calibrate** menu to open the Display Calibration Graphs dialog.



2. Select the Static, Scanning, or Scan Speed Compensation calibration type.

3. Use the default, or click **Browse**, and select a file.

   The default files are STAT.RAW for the static file, SCN.RAW for scanning, and FAST.RAW for scan speed compensation.

4. Optionally, enter a range of scans to combine **From** and **To**.

5. Click **OK**.

Recalibrating a Data File

This option allows the current calibration to be applied to a previously acquired data file.

1. Select **Recalibrate Data File** from the Calibration **Process** menu to open the Display Calibration Graphs dialog.

2. Click **Browse** and select the data file you want to recalibrate.

3. Click **OK**.

Editing a Reference File

The table below lists the contents of the file Hepta.ref that is the standard reference for EI calibration. Calibration reference files consist of two columns of numbers separated by any number of spaces or TAB characters. The first column contains the reference peak masses; the second column contains the reference peak intensities. The reference peak intensities are not at present used by the calibration software and so can be set to a nominal value of 100. However, you may wish to enter realistic values here to improve the appearance of the reference spectra.

49.99379	0.73
68.99518	100.00
99.99358	6.31
118.99199	7.80
130.99199	36.31
149.99039	1.29
168.98877	3.24
180.98877	1.31
218.98560	38.07
263.98705	8.38
313.98386	0.32
375.98067	0.38
413.97748	1.64
463.97429	1.02
501.97110	1.90
537.97112	0.13
575.96796	0.32
613.96471	0.64

You can create or edit calibration reference files using any Windows text editor. To read the currently selected reference file into the Notepad text editor, select **Reference File** from the Calibration **Edit** menu.

After editing, the reference file can either be saved under the current name by selecting **Save** from the Notepad **File** menu, or saved as a new reference file by selecting **Save as** from the Notepad **File** menu and giving the file a new name.

Textual information or comments can be stored in the reference file. Lines, which are textual information or comments, must start with a semi-colon ; character.

High Mass Calibration

Heptacosa's highest mass peak for calibration is m/z 614. Calibrating to higher mass requires a different compound that has ions at higher m/z.

One compound useful for this purpose is Tris(perfluoroheptyl)-s-triazine, found in the mass calibration file Triazine.ref.

This compound has calibration ions up to m/z 1185. It is soluble in methanol and hexane, has a low boiling point, and may be chromatographed easily.

Performing a High Mass Calibration

1. Calibrate as usual to Heptacosa.
2. Change the reference file from helpta to Triazine.
3. Inject 0.2 *n*L of the triazine compound splitless into a 250º C injector with a 30 m x 0.25 mm x 0.25 *n*m column at 80º C. Program to 300º C at 10º /min.
4. When the major portion of the peak begins to elute at *n*6 minutes, start the calibration process.
5. Open the split valve after calibration is completed.
6. Perform a wet-needle injection of this compound in splitless mode and acquire a data file over the desired mass calibration range.

   This will drastically overload the GC column, and provide several seconds of high-intensity ions.
7. Use the **From File** option in the **Process** menu, select **Scan Speed Compensation**, and select your data file with the **Browse** function.
8. Click **OK** to calibrate.
9. Inspect the calibration to verify correctness.

   Make manual identifications, if required.

For SIR, start a **Static**-only mass calibration as soon as you see the target peaks in the Tune display.

For a full-scan analysis, perform a **Scanning**, and then a **Scan Speed Compensation** calibration as described above for **Static**. An alternative for full-scan calibration is to create a simultaneous two-function acquisition method with two different scan times – one for the **Scanning**, and one for the **Scan Speed Compensation**.

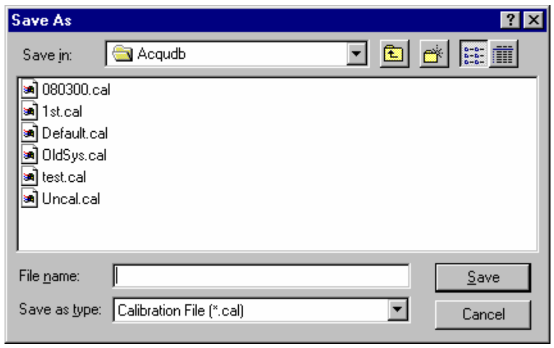
Saving and Restoring Calibrations

The complete instrument calibration can be saved to disk as a named file and then recalled at a future date. Static, dynamic, and lag-time calibrations are all saved together under a common name.

You may find it useful to calibrate the instrument for each of the different types of experiments that you do and save these calibrations to disk. This means that when you switch between experiments, you can restore a suitable calibration from disk rather than having to recalibrate from scratch.

Saving a Named Calibration

1. Click **Save As** from the Calibration **File** menu, and enter a new file name.



2. Click **Save**.

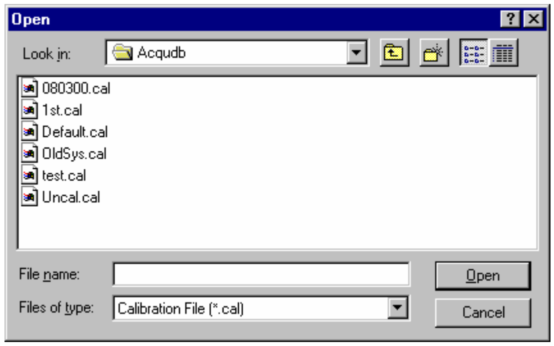
   If the selected file exists, you will be asked to confirm that you want to overwrite the existing information. Click **OK** to continue or **Cancel** to enter a different file name.

Restoring a Saved Calibration

1. Select **Open** from the Tune **File** menu.

2. Select the calibration file required, either by entering its name or by selecting it from the displayed list.

3. Click **Open** to display the Load Instrument Calibration dialog.



4. Select the desired calibration file.

5. Click **OK**.

GC Control 7

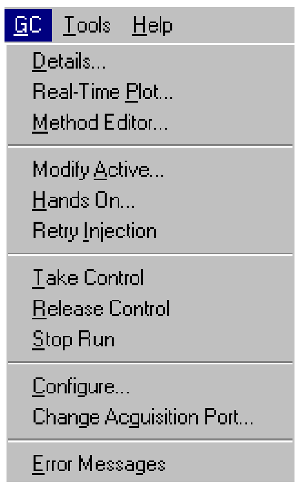
Overview of TurboMass GC Control

This section contains the software procedures required for GC control when the PerkinElmer Clarus 500 GC or AutoSystem XL GC is used as the inlet for the mass spectrometry system.

You need to configure the mass spectrometer for GC control and develop your GC method before you execute your MS method.

The GC Menu

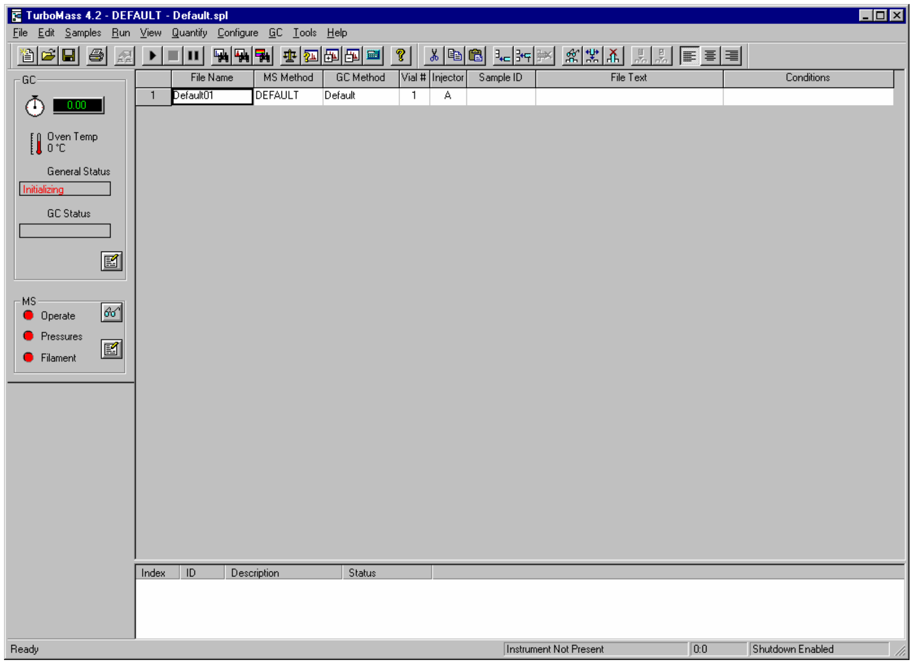
All GC commands are located in, or are accessible from, the **GC** menu in the TurboMass top level window and Sample List. From the **GC** menu you set up your GC configuration, develop your GC method, work interactively with the GC, and perform all other GC related procedures.



The GC Status Box

You can monitor the GC status from the TurboMass top level window GC Status box. The GC Status box displays the GC oven temperature and the general GC status. The general GC status indicates the run status or the GC operational status.

For information on GC status messages, see *Understanding GC Status Messages* on page 185.



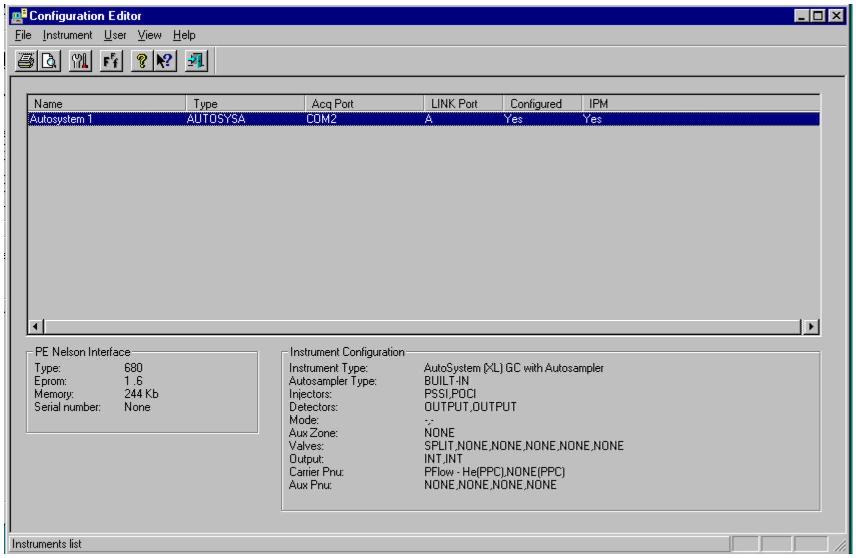
The GC Editor Toolbars and Status Bars

There are two GC editors, the Configuration Editor and the Method Editor. Each GC editor has a toolbar with buttons that give you quick access to commonly used commands. When you point to a toolbar button, a tool tip will appear beneath the button as well as a definition in the status bar at the bottom of the window. The toolbar is displayed by default. You can hide the toolbar by selecting **Toolbar** from the **View** menu in both GC Editors.

A status bar appears at the bottom of each GC editor that displays a short Help message explaining the function of the command you highlight in a menu, or the button that the mouse is positioned over. The status bar is displayed by default. You can hide the status bar by selecting **Status Bar** from the **View** menu in both GC Editors.

Configuration

When you open the Configuration Editor the screen displays information defined during configuration.



Name	Your name for the GC.
Type	The GC model or type.
Acq Port	The physical data acquisition port to which the 600 Series LINK Interface is connected.
LINK Port	The physical port to which the GC is connected.
Configured	Displays **Yes** if you have provided all the information TurboMass needs to configure the GC. Otherwise, the status is **No**.

IPM	Shows whether or not the Instrument Personality Module (IPM) for the GC has been downloaded. The first time you open this window, the IPM will not have been downloaded. Once configuration is complete, the area below the Configuration Editor Summary list displays key GC information. On the left is information about the LINK interface including the type (model number), EPROM version number, memory size available in the interface (in bytes), and serial number. On the right is a summary of the GC configuration.

Configuring TurboMass for GC Control

The procedure used to configure the GC depends upon whether you are initially configuring TurboMass for GC control or are making changes from the GC keypad.

Initial GC Configuration - Use to set up the LINK and GC for TurboMass control for the first time.

Reconfiguring the GC - Use to make changes from the GC keypad or hardware changes to the GC without changing the LINK configuration. Reconfiguration is also required if you add an autosampler.

Initial GC Configuration

There are four steps to configuring TurboMass for GC control for the first time:

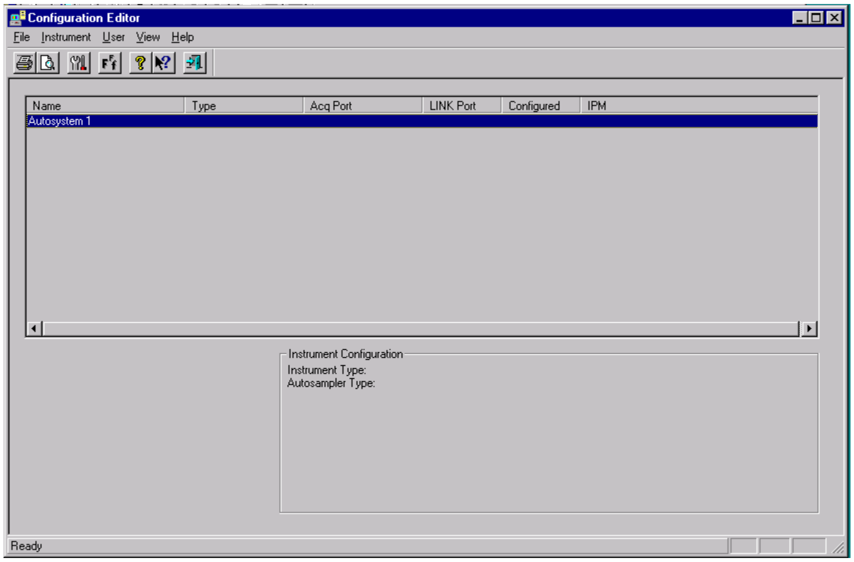
- Confirm a data acquisition port.
- Confirm the LINK configuration.
- Set the GC configuration options.
- Save the configuration.

Each step is described in a separate procedure.

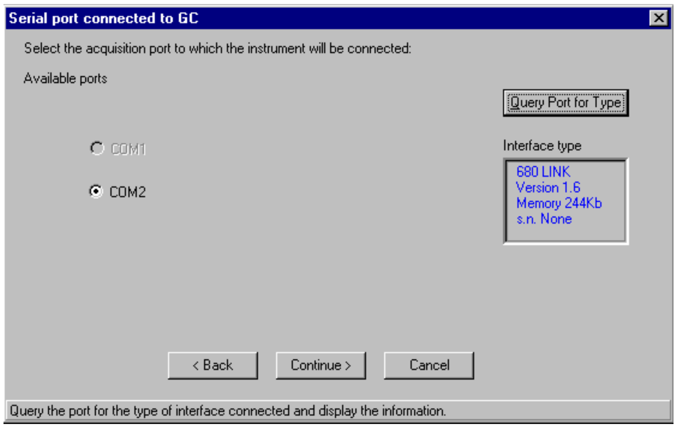
Confirming a data acquisition port

1. Open the TurboMass application to display the TurboMass top level window.

2. Select **Configure** from the **GC** menu to open the Configuration Editor.

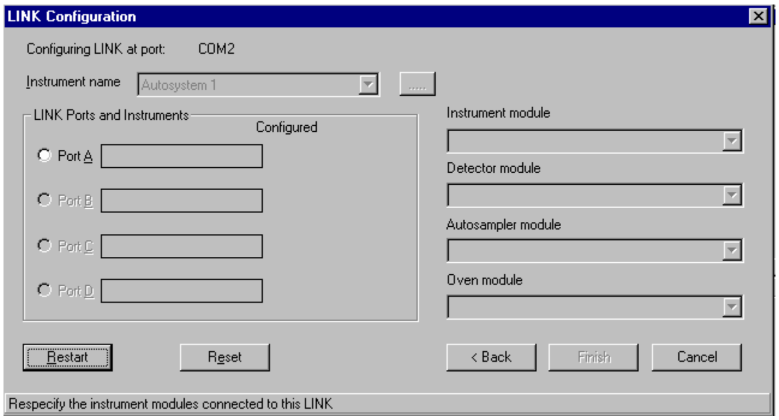


3. In the Configuration Editor, select **Configure** from the **Instrument** menu to open the Serial port connected to the GC dialog.



4. Select the serial port and click **Continue**.

   The LINK Configuration dialog displays the COM port and instrument name.



Confirming the LINK configuration

1. Select the **LINK** port for the GC.

   For an integral Link, you must select Port A.

2. Select AutoSystem With or Without Autosampler or Clarus 500 With or Without Autosampler in the Instrument module drop-down list, according to your GC configuration.

You must select **AutoSystem With Autosampler** or **Clarus 500 With Autosampler** if an autosampler is installed on your GC. You may exclude use of the autosampler in the GC Method Editor.

If you make a mistake, click **Restart** to disconnect the GC and clear the **LINK** port. Click **Reset** to clear all changes and return this dialog to the state it was in before it was opened.

Setting the GC configuration options

1. In the LINK Configuration dialog, click **Configured** (next to the port selection) to open the GC Configuration dialog.

2. To rename the GC to something other than its default name, enter the new name in the **Name** field.

3. Under **Options**, select whether or not you have PPC (Programmable Pneumatic Control) installed.

   Selecting **YES** activates the other PPC options.

4. Under **Inlets**, select the Injector setting that matches your GC for Channel A and/or B.

5. Select the valve type for each valve in the GC.

   The PPC split vents will be configured automatically.

6. Select PPC for detector A and/or B if detectors and PPC are installed.

7. Under **Detectors**, select the **Detector**, **Mode**, and **Output** settings that match any additional detectors installed on your GC for Channel A and/or B.

8. Under **Carrier Pneumatics**, select the **Pressure units** and other options.

9. Select a setting for **Carrier A**.

   PVel Denotes *programmable* linear velocity operation. This option is only available for CAP and PSSx injectors in Cap Control Mode. (You enter the average values for capillary column linear velocity in the method, as well as values for column dimensions

and vacuum compensation.)

CFlow Denotes operation at a *constant* flow rate. (Enter pressure values in the method.) The pressure is varied by the GC to maintain a constant mass flow rate through the column as the oven temperature changes. This mode does not require you to enter column dimensions in the method.

PFlow Denotes *programmable* flow operation. (Enter flow values in the method.)

Press Indicates direct pressure *programmable* control in the pressure units you select.

IFlow Denotes *constant* flow operation. (Enter flow values in the method.)

10. If appropriate, repeat the process for **Carrier B**.
11. Under **Auxiliary Pneumatics**, select PPC for any auxiliary zone that has a PPC controller installed.
12. Select the settings to control pressure or flow of the auxiliary zone(s).
13. Click **OK**.

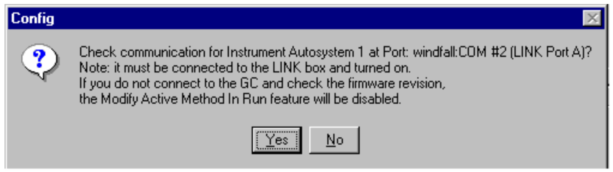
    A check mark in the LINK Configuration dialog indicates that the GC has been configured.

Saving the configuration

1. Click **Finish** in the LINK Configuration dialog to save the configuration.

   TurboMass creates a configuration file (.CFG) for the GC and downloads the appropriate IPM. The IPMs available to you are installed during TurboMass installation.

   When you first configure the GC, the Config message appears:



2. If the GC is connected and turned on, click **Yes**.
3. TurboMass will attempt to check the physical connection with the GC by taking, and then releasing, control of the GC.

   The Confirm Configuration message appears.

4. To compare the configuration options you selected with those that are being reported by the GC, click **Yes**.

   A series of confirmation messages appear.

5. Respond to each message.

   When TurboMass is finished, the Configuration Editor appears.

   Yes appears in the Configured column if your LINK and GC are adequately configured. If **No** appears, you need to complete the configuration before you can acquire data.

Reconfiguring the GC

If you make hardware or other configuration changes to your GC after you have configured TurboMass for GC control, you can reconfigure the GC settings without changing the LINK configuration.

However, if you add an autosampler to a GC, you must reconfigure the LINK and GC as you did when you initially configured your GC. As you are starting with a configured LINK and GC, you must first disconnect the GC from TurboMass control and clear the LINK configuration.

1. In the TurboMass top level window, select **Release Control** from the **GC** menu to release TurboMass control of the GC.

   Releasing the GC from TurboMass control lets you control the GC from the keypad. The GC front panel display changes from “External” (TurboMass) to “Method#” control, where Method# is an internal GC method.

2. Make the required changes from the GC keypad.

3. To update your GC configuration in the TurboMass Configuration Editor, select **Configure** from the **Instrument** menu to open the GC Configuration dialog, and either click **Query Inst for Config** to obtain your updated parameters from the GC, then click **OK**.

   OR

   Enter your changes in the GC Configuration dialog, and click **OK** to update your GC configuration.

For more information on setting the GC parameters, see *Setting the GC configuration options* on page 147.

Changing the Instrument Configuration

1. Select your instrument in the Configuration Editor.

2. Select **Disconnect** from the Configuration Editor **Instrument** menu, respond to the confirmation message that appears, and click **OK**.

   TurboMass clears your LINK port and GC configuration information.

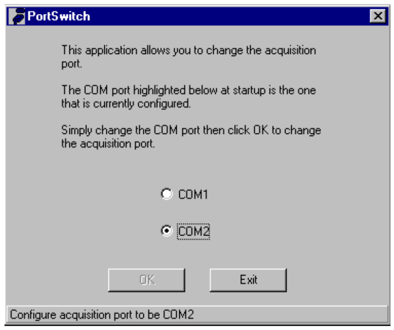
3. To reconfigure your LINK and GC to reflect your new instrumentation, see *Configuring TurboMass for GC Control* on page 144.

Changing Your Acquisition Port

You can change the serial port without reconfiguring your LINK and without opening the Configuration Editor. Before starting this procedure, be sure to reconnect the serial cable to the appropriate port on your PC.

1. Select **Release Control** from the **GC** menu to release the GC from TurboMass control.

2. Select **Change Acquisition** Port from the **GC** menu to open the PortSwitch dialog.



3. Select the appropriate port, and click **OK**.
4. In the **GC** menu, select **Take Control** to re-establish (TurboMass) control of the GC.

   TurboMass changes the selected COM port and updates your configuration.

Configuring TurboMass without GC Control

You can configure TurboMass for data reprocessing only or for use with a GC that is not under TurboMass control.

1. Select **Configure** from the **GC** menu to open the Select Interface dialog.
2. To configure TurboMass, for data reprocessing only, select **None**

   OR

   For data acquisition but not GC control, select **Contact Closure**.

Configuring User Options

From the Configuration Editor **User** menu, you can change the fonts used to print out the GC method summary and you can set up quick paths.

Changing Fonts

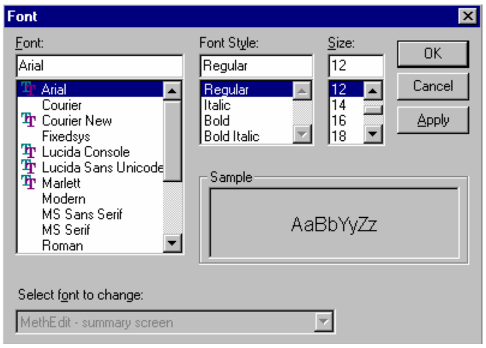
The Font dialog lets you choose the typeface, style, and size of text that will appear in the Method Editor Summary.

Selecting a Font

1. To open the Font dialog, select **Fonts** from the **User** menu

   OR

   Click the fonts tool.



   The Method Editor Summary is automatically selected in the **Select font to change** drop-down list.

2. Select a **Font**, **Font Style**, and **Size** of text.

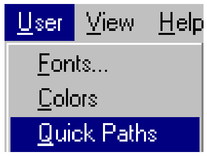
3. Click **OK**.

Specifying Quick Paths

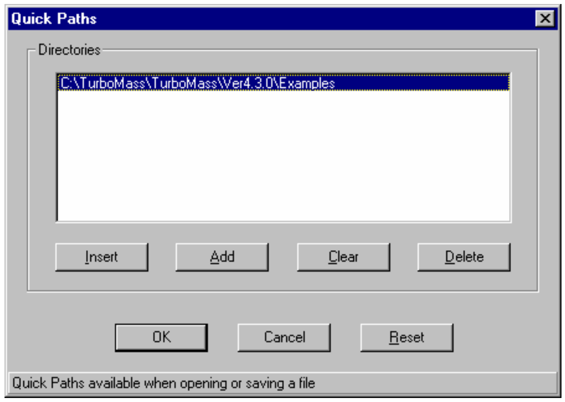
Specifying a quick path lets you quickly choose a frequently used path in any file selection dialog in the GC editors. This provides, for example, immediate access to your mass spectrometry project file, instead of scrolling and clicking through the Windows file-selection method.

Adding a path to the Quick Paths list

1. In the Configuration Editor, select **Quick Paths** from the **User** menu.

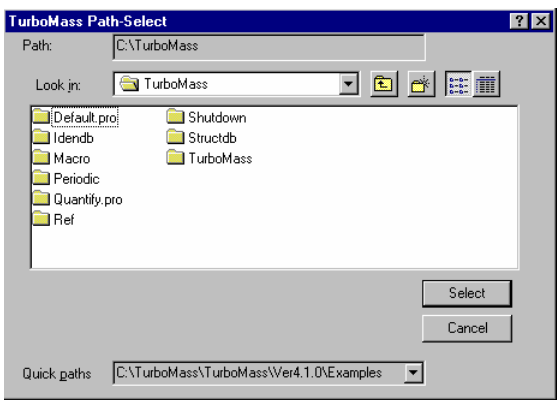


The Quick Paths dialog box appears and lists the current quick paths.



2. Click **Add**.

The TurboMass Path-Select dialog opens:



3. Select a path and click **Select**.

   TurboMass will add the path as a quick path and list it in the Quick Paths dialog.

   If you want to set a quick path to your project directory, specify the following quick path to the project subdirectory that contains the GC method:

   <project path>\acqudb

   For example:

   c:\TurboMass\myproject.pro\acqudb\

   If you do not specify a project directory, TurboMass creates the following project directory as a default, which you can specify as one of your quick paths:

   c:\TurboMass\Default.pro

Inserting a path in the Quick Paths list

1. In the Configuration Editor, select **Quick Paths** from the **User** menu to open the Quick Paths dialog.

2. Select the path above which you want to insert a new quick path, and click **Insert**.

3. In the Path-Select dialog select a path, and click **Select**.

   TurboMass will add the path to the Quick Paths list.

Removing a quick path from the Quick Paths list

1. In the Configuration Editor, select **Quick Paths** from the **User** menu to open the Quick Paths dialog.

2. Select the path you want to delete from the Quick Paths list, and click **Delete**.

Removing all paths from the Quick Paths list

1. In the Configuration Editor, select **Quick Paths** from the **User** menu to open the Quick Paths dialog.

2. Click **Clear**.

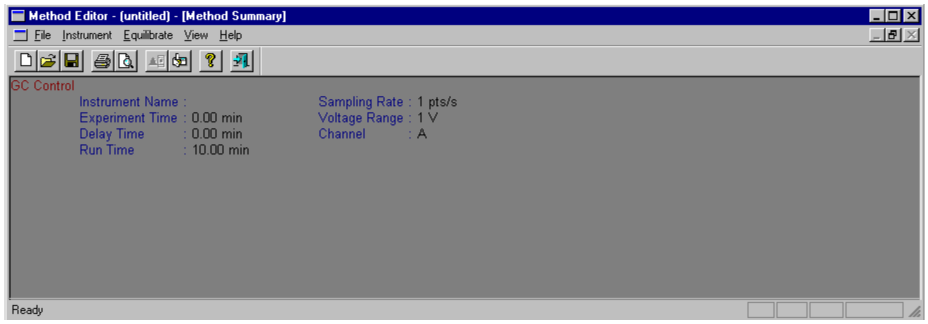
3. If you change your mind, click **Reset** to replace the original paths.

Printing Configuration Information

The **Print** command in the **File** menu lets you print a copy of the LINK and GC configuration information. Configuration information includes font choices, quick paths, and GC and interface data.

GC Method Editor

You use the Method Editor for all GC method operations. When opening the Method Editor from the **GC** menu, the Method Summary Window is displayed.



The Method Summary Window contains the data acquisition and GC control information including the run-time information and control options, such as injector temperatures, carrier gas settings, and oven program.

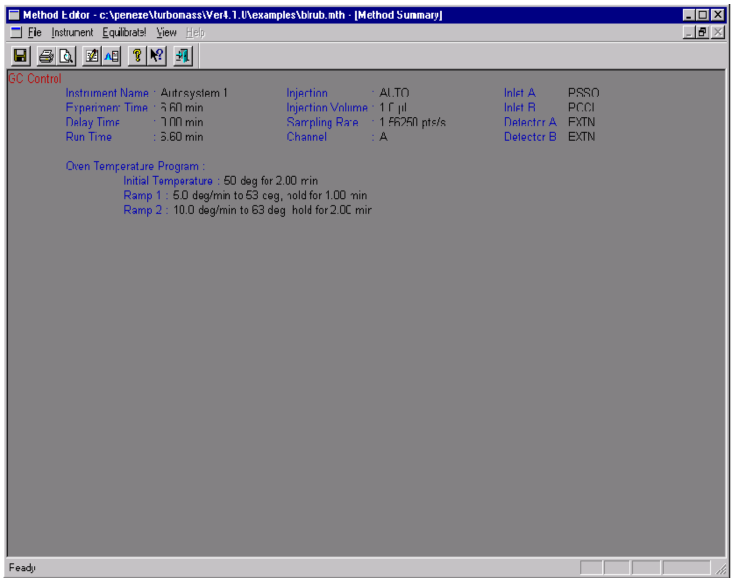
Developing a GC Method

To develop a new GC method, set data channels, and set your GC control options.

You can also create a new method by editing an existing method file and renaming it with the Save As Command.

Creating a new GC method

1. Select **Method Editor** from the **GC** menu in the TurboMass top level window
   OR
2. Click  in the GC panel.
3. Select **Create new method** in the Startup dialog, and click **OK** to open the Method Editor.



Opening an existing method

You can open an existing method from two places:

- From the Method Editor:

  ➢ Select **Method Editor** from the **GC** menu to open the Startup dialog.

  In the Startup dialog, select **Load method stored on disk**, or select **Load recently edited method** and select the desired method.

- From the Sample List:

  ➢ Right-click the Inlet File cell in the Sample List that contains the GC method you want to open, and select **Open** from the drop-down menu

  OR

  Select **Open** from the TurboMass **Edit** menu.

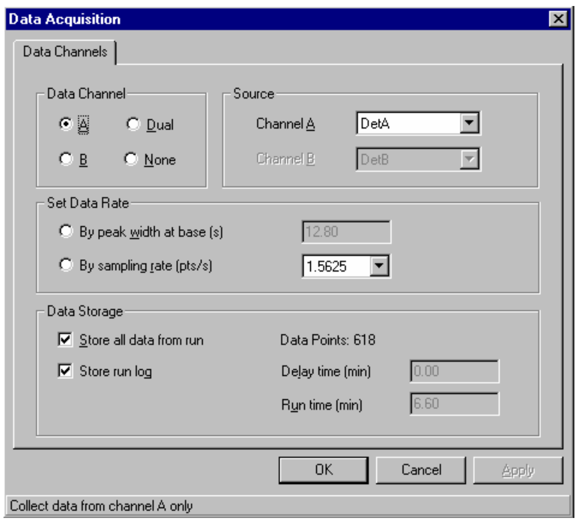
Setting Data Channels

The **Data Channels** command in the **Instrument** menu control how TurboMass acquires analog and digital data by letting you set the channel or channels for data collection, the data sampling rate, and the analysis run time. Some of the options available on the Data Channels tab depend on the type of instrument that you are using. If not, select **None**.

NOTE: *Setting data channels applies only if you have additional conventional detectors installed on the GC. If not, choose "None."*

Setting channel options for the GC

1. Select **Data Channels** from the GC Method Editor **Instrument** menu to open the Data Acquisition dialog.



2. Under **Data Channel**, select channel **A**, **B**, **Dual**, or **None**.

3. Under **Source**, select the appropriate additional signal source for the data channel(s).

4. Under **Set Data Rate**, to set the rate at which the GC will sample its detectors either select **By peak width at base**, and then enter the number of seconds in the text field.

   With this option, TurboMass acquires data in terms of the width (at its base) of the narrowest peak that you expect to occur in the run. If you enter a peak width, TurboMass calculates the optimum sampling rate for that peak width, collecting at least 20 data points across the peak.

   OR

   Select **By sampling rate**, and then enter or select a rate.

   With this option, TurboMass acquires data from the GC using the number of data points per second that you explicitly set (or the nearest available rate to that value).

5. Under **Data Storage**, either select **Store all data from run** to store all the data from a run.

   This option is useful if you don't know the run time because you have not entered the GC oven program.

   OR

   Deselect **Store all data from run** to store only the data collected in a given time window.

   You must specify the relevant times. In the **Delay time** field, enter the number of minutes that you want to elapse between the start of the run and when data analysis starts. In the **Run time** field, enter the number of minutes for which you want the interface to collect data. Note that the run time must always be greater than the delay time.

6. Select **Store run log** to upload the run log at the end of each run.

   When you select this option, TurboMass prints the GC run log as part of the report. **Store run log** is available even when there are no additional detectors installed on the GC.

7. To save your work and close the dialog, click **OK**.

Setting Control Options

The **Control Options** command in the **Instrument** menu opens a submenu that has additional commands for controlling your instruments. When you select a command from this submenu, TurboMass opens the Instrument Control dialog, which contains tabs for each major control command.

Setting control options parameters

1. Select **Control Options** from the **Instrument** menu and select a command from the cascaded menu.

   The Instrument Control dialog opens to the tab corresponding to the command that you selected.

2. Select the tab for each control option that you want to complete or edit.

3. Make any changes to the values in the dialog.

4. To save your work and close the dialog, click **OK**

   To save your work without closing the dialog, click **Apply**

   To close the dialog and discard your changes since the last time you clicked **Apply**, click **Cancel**.

The following sections describe how to complete each of the tabs in the Instrument Control dialog.

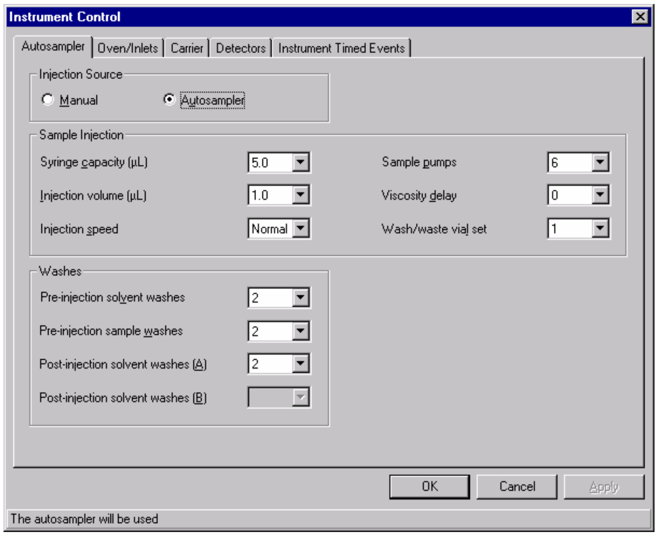
The possible tabs in the Instrument Control dialog are:

- Autosampler.
- Oven/Inlets.
- Carrier.
- Valves.
- Detectors.
- Instrument Timed Events.

For a complete definition of each GC parameter, refer to your *GC hardware manual*.

Setting autosampler parameters for the GC

1. Select the **Autosampler** tab of the Instrument Control dialog.



2. If you are using manual injection, select **Manual**

   OR

   If you are using an autosampler, continue with Steps 3 through 9.

3. Select the **Syringe capacity** for the syringe in the autosampler.

4. Select the actual Injection volume and an Injection speed.

5. Select the number of **Sample pumps** that you want to use.
   This value specifies the number of times the syringe is filled and emptied before the final load.

6. If you are injecting a viscous sample, set the **Viscosity delay**.

7. Select the **Wash/waste vial set** that you want to use.
   Wash/waste vial set 1 uses vials 1 and 2. Wash/waste vial set 2 uses vials 3 and 4.

8. Select the number of **Pre-injection solvent washes** that you want to have.

   This value determines how many times the syringe is washed with solvent before each injection.

9. Select the number of Pre-injection sample washes and Post-injection solvent washes that you want to have.

Setting GC Oven/Inlets Parameters

The Oven/Inlets tab of the Instrument Control dialog controls the oven temperature of your gas chromatograph, the rate at which the temperature increases, the type of coolant that you are using, and the zone setpoints for injectors and detectors.

The Ovens/Inlets tab also includes a temperature curve that corresponds to the values that you enter in the table beneath it. The table has the following columns:

Rate Represents the rate at which the oven is heated. You can create up to three ramps, which are periods during which the temperature increases. Ramps are in degrees per minute.

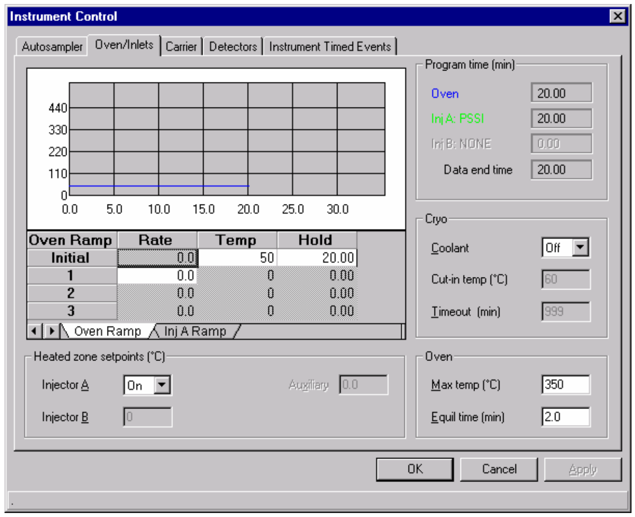
Temp Gives the temperature to which the oven is being raised during the ramp.

Hold Represents the period for which the temperature is held before starting the next ramp. The initial setting is the temperature of the oven at the start of the run, or throughout the run for an isothermal analysis.

The **Initial Rate** field is always 0.0 and you cannot edit this field. To edit the other fields, click in the field and then enter a value. The Temperature and Hold fields are disabled until you set the Rate.

You can also adjust the Temperature and Hold values by dragging the corresponding points on the curve to the desired position.

1. Select the **Oven/Inlets** tab of the Instrument Control dialog.



3. From the available program tabs beneath the table, select the tab for the temperature program that you want to edit.

   The curve for the program that you select appears as a solid line. The curves for all other programs appear as dashed lines.

4. In the **Initial Temp** field of the table, set the temperature for the start of the run.

5. In the **Initial Hold** field, enter the amount of time that you want to hold the initial temperature.

   To hold the temperature until the end of the oven program, enter 999.

6. Set the **Rate**, **Temp** and **Hold** values for the other ramp levels.

   The time value under **Program time** changes to reflect the time that is required to complete the temperature program.

7. You can also change the values directly on the curve by dragging the points associated with each ramp level. When you release the points after dragging, the new values appear in the table.

   - To change the rate of a level, select the point that represents the temperature and drag it horizontally.

   - To change the temperature value of a level, select the point that represents the temperature and drag it vertically.

   - To change the hold time duration of a level, select the point that represents the time and drag it horizontally.

8. Under **Cryo**, select the type of sub-ambient cooling that you want to use, or set **Coolant** to **Off**.

9. If you are using sub-ambient cooling, enter the values for the cryogenic **Cut-in temperature** and the oven **Timeout** in the respective fields.

10. Under **Oven**, enter the maximum oven temperature allowed.

    This value protects the installed column.

11. In the **Equil time** field, enter the number of minutes that you want the oven to equilibrate at the initial temperature before it becomes READY.

    For temperature programming (ramping), set the Equil Time to at least 2 min.

12. Under **Heated zone setpoints**, if you have non-programmable inlets enter the temperature for **Injector A** and **Injector B**.

    If you have programmable inlet type POC or PSS configured in either inlet program mode or oven tracking mode POCI, PSSI, POCO, or PSSO, select either **On** or **Off** for Injectors A and B.

    POCO and PSSO track the oven program temperature +5 °C.

13. If the option is available, enter an **Auxiliary** zone temperature.

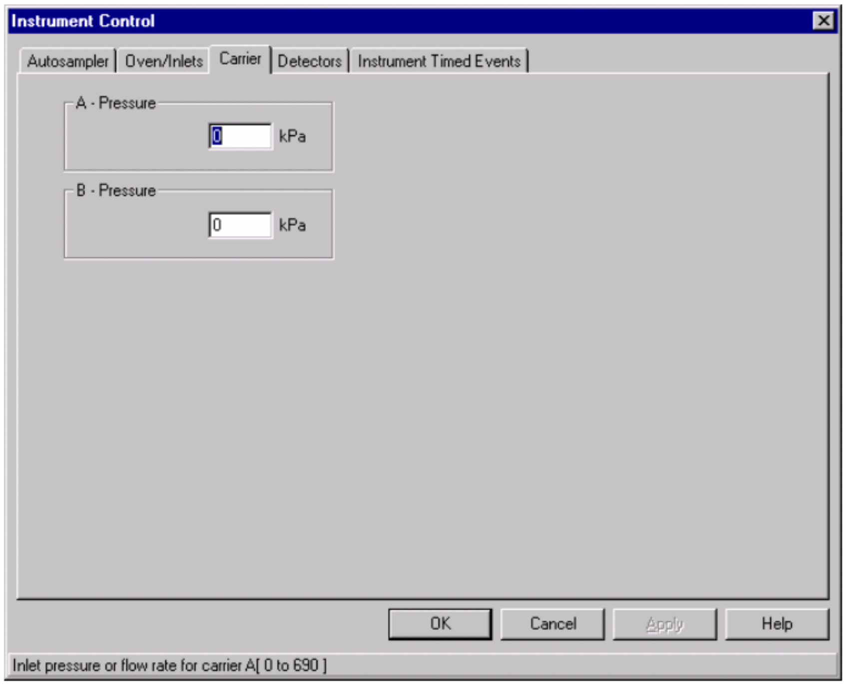
Setting GC Carrier Parameters

You can use the Carrier tab of the Instrument Control dialog to set carrier parameters such as the inlet pressure or flow rate for carrier gas.

If the GC has neither carrier nor auxiliary zone configured as a PPC Zone, you can enter only the pressure and flow values for inclusion in the instrument's Ready logic. You must set the actual pressure and flow rate on the GC itself.

Setting carrier parameters without PPC zones

1. Select the **Carrier** tab of the Instrument Control dialog.



2. Enter the **Pressure** or flow rate for carrier A and B.

   Enter 0.0 if you do not want the actual pressure or flow setting to prevent the instrument from becoming ready.

Setting GC Carrier Parameters with PPC Zones

If the GC has either carrier or any auxiliary zones as a PPC zone, you can enter information about the column, program, inlet split controls, and auxiliary pneumatics setpoints.

The Carrier tab also includes a pressure/flow/velocity curve that reflects the values that you enter in the table beneath it. You can switch among different carrier programs by selecting the program tabs at the bottom of the table. The table has the following columns:

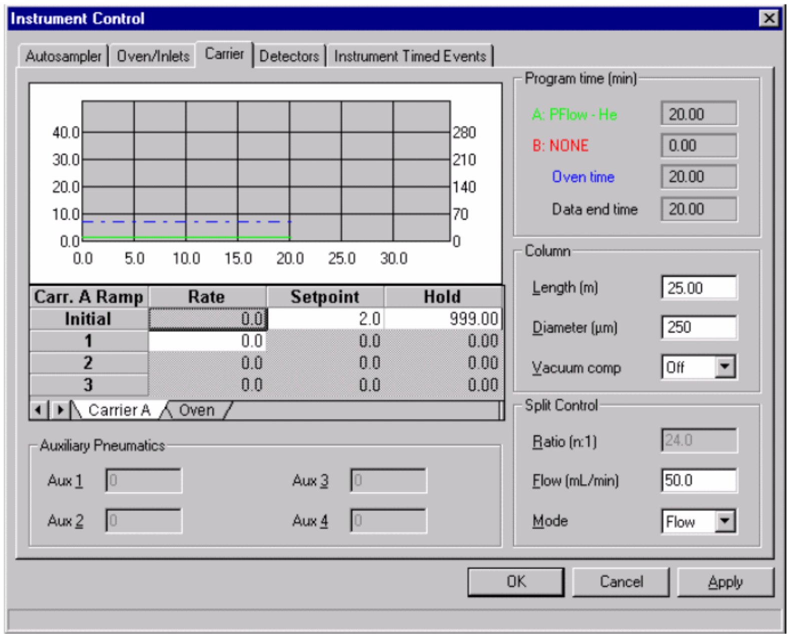
Rate Represents the rate at which the carrier pressure/flow/velocity changes. You can create up to three *ramps,* which are periods during which the pressure/flow/velocity changes. Ramps are shown on the vertical axis of the curve.

Setpoint/Temp Gives the pressure/flow/velocity to which the carrier is being changed. When **Oven** is selected, it displays the temperature for the oven.

Hold Represents the period for which the pressure/flow/velocity is held before starting the next ramp. The initial setting is the pressure/flow/velocity of the carrier at the start of the run, or throughout the run.

The **Initial Rate** field is always 0.0 and you cannot edit this field. To edit the other fields, click in the field and then enter a value. The **Setpoint** and **Hold** fields in a ramp are disabled until you set the **Rate**.

1. Select the **Carrier** tab of the Instrument Control dialog.



2. From the available program tabs beneath the table, select the tab for the program that you want to display.

   The curve and the table change to reflect the program that you select. The curve for the program that you select appears as a solid line. The curves for all other programs appear as dashed lines.

   The information under **Program time** also changes to reflect the selected carrier values. The color-coded carrier time fields show how much time is required to complete the pressure/flow/velocity program. Aux Time appears instead of the carrier time for certain instruments. **Oven time** shows how much time is required to complete the oven program.

3. In the **Initial Setpoint** field of the table, set the flow/pressure/velocity for the start of the run.
4. If the program you are editing is a constant flow/pressure/velocity program, then you can only enter an initial **Setpoint** value in the table.

5. In the **Initial Hold** field, enter the length of time to hold at the final flow/pressure/velocity for this program step.

   To hold the flow/pressure/velocity until the end of the temperature program, enter 999.

6. Set the **Rate**, **Setpoint** and **Hold** values for the other ramp levels.

7. You can also change the values directly on the curve by dragging the points associated with each ramp level. When you release the points after dragging, the new values appear in the table.

   - To change the rate (flow/pressure/velocity) of a level, select the point that represents the setpoint and drag it horizontally.

   - To change the setpoint value of a level, select the point that represents the setpoint and drag it vertically.

   - To change the hold time duration of a level, select the point that represents the time and drag it horizontally.

8. If you selected capillary mode during instrument configuration, set the **Length** and **Diameter** of the column under **Column**.

9. Turn on the **Vacuum compensation** for the column.

10. If the instrument is configured with auxiliary pneumatics, enter the **Auxiliary Pneumatics** setpoints for any auxiliary zones.

11. Under **Split Control**, select a split control mode.

12. If you select **Ratio**, enter a split ratio in the Ratio field.

    OR

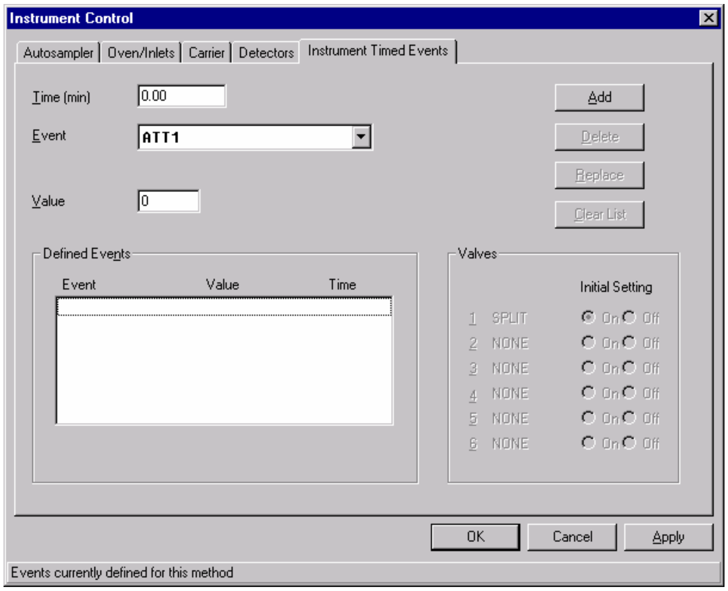
    If you select **Flow**, enter a split flow in the Flow field.

Setting GC Valves

You can use the **Instrument Timed Events** tab of the Instrument Control dialog to enter the initial settings for any valves installed on the GC.

1. Select the **Instrument Timed Events** tab of the Instrument Control dialog.

   The **Valves** group reflects the system configuration.



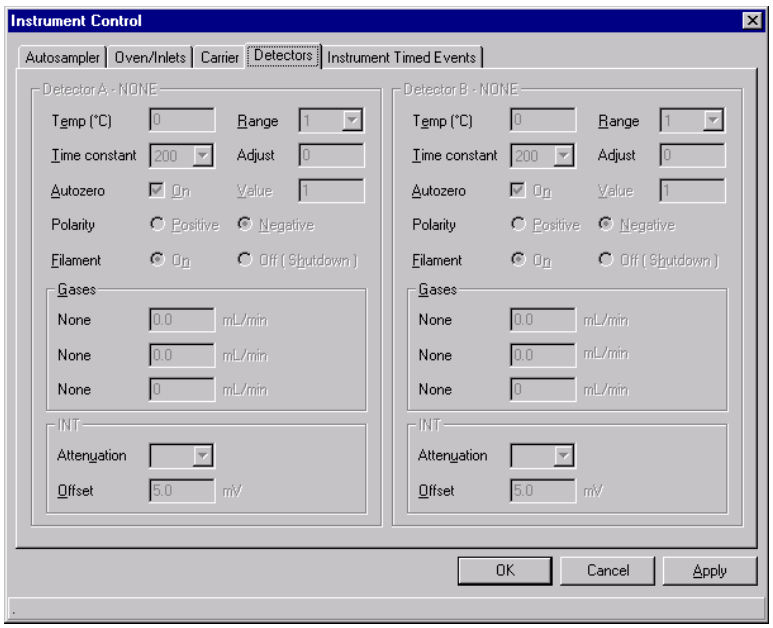
2. Under **Valves**, set the **Initial Setting** buttons to **On** or **Off** for each valve.

Setting GC Detector Parameters

NOTE: *These parameters apply only if you have additional conventional detectors installed on the GC.*

You can use the Detectors tab of the Instrument Control dialog to control the sensitivity of detection during the analysis as well as the magnitude of any optional analog output from the GC.

1. Select the **Detectors** tab of the Instrument Control dialog.



2. In the **Temp** field, enter a temperature value for the detector.

3. Select a sensitivity setting for the detector from the **Range** drop-down list.
4. This value is the gain level of the detector output. The values depend on the instrument and detector type. For example, if you are using a Clarus with an FID, the lower the Range setting, the greater the detector sensitivity. For a TCD, the lower the Range setting, the lower the detector sensitivity.

5. Select a Time constant.

   This value sets the detector filter width in milliseconds, which smoothes out the detector signal. Higher values improve the signal-to-noise ratio but attenuate narrow peaks.

6. If you are using an FPD detector, set the **PMT %**.

   This value is the percentage of the maximum photo-multiplier voltage and sensitivity.

7. To make the detector autozero at the start of each run, select **Autozero On**.

8. If the **Value** field is available, enter a value to specify an offset.

9. If the **Polarity** option is available, select **Positive** or **Negative**.

10. If the **Filament** option is available, select **On** or **Off**.

11. Under **Gases**, specify the gas flow rates for the detector.

12. If the GC configuration includes either REC (Recorder) or INT (Integrator) settings for analog output, set the following options under REC or INT:

    - Select an **Attenuation** value for analog output from the **Attenuation** drop-down list.

    - In the **Offset** field, enter the amount by which to offset the analog output for an external recorder.

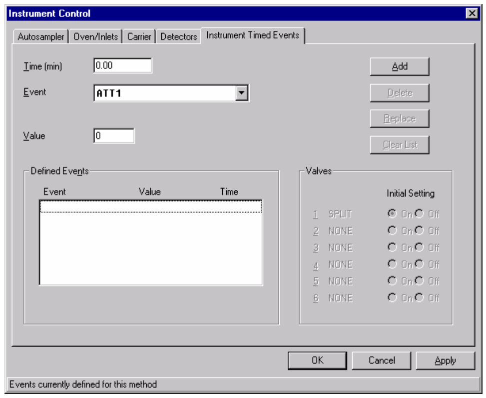
14. Repeat Steps 2 through 11 for the second detector.

Setting Instrument Timed Events

Use the Instrument Timed Events tab of the Instrument Control dialog to select one or more timed events from a predefined list, and enter the time at which you want the event to take place.

Adding or editing timed events

1. Select the **Instrument Timed Events** tab of the Instrument Control dialog.



2. In the **Time** field, enter the time at which you want this event to occur during the run.

3. From the **Event** drop-down list, select the event that you want to add.
4. If the event requires a value or setting, the **Value** field becomes enabled.

5. Depending on the event, use the **Value** field or list to specify a value for the event.

6. Click **Add** to add this event to the **Defined Events** list.

7. Repeat Steps 2 through 5 to add other events.
   TurboMass list the events in the order of the time at which they occur.

Changing the time or value of a timed event

1. Under **Defined Events**, select the event that you want to change.

2. To change the time, enter a new number in the **Time** field.

   OR

To change the value, either select one from the list or enter a value in the field.

3. Click **Change**.

Deleting a timed event

1. Under **Defined Events**, select the event that you want to delete.

2. Click **Delete**.

Deleting all timed events

Click **Clear**.

Entering Descriptive Information for GC Files

From the Method Editor you can enter descriptive information about your GC method and/or enter audit trail information.

You may enter descriptive information about a method on the **Description** tab of the Documentation dialog, and you may enter information about changes made in the Audit Trail dialog (if auditing is enabled.) One or the other will appear automatically when you save a file according to the following rules:

- The **Description** tab in the Documentation dialog always appears when you save a new file. If auditing has not been started for a file, then the Description tab also appears when you use Save As to save an existing file with a new name.

- If auditing has been started for a file, the Audit Trail dialog appears every time you save that file with either Save or Save As.

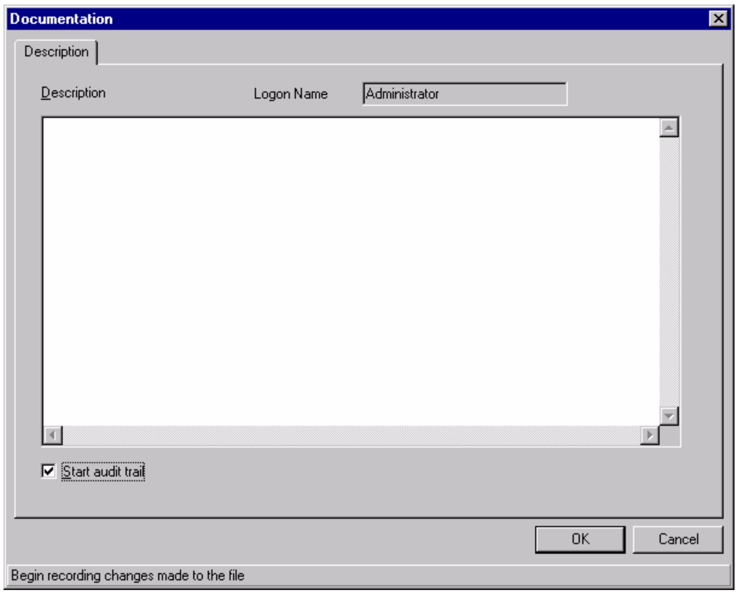
You enable an audit trail by selecting **Start audit trail** on the **Description** tab. Once an audit trail is started, the Description dialog will not appear automatically if you select **Save As**. However, you can display it at any time by selecting **Description** from the **File** menu.

The Description tab in the Documentation dialog

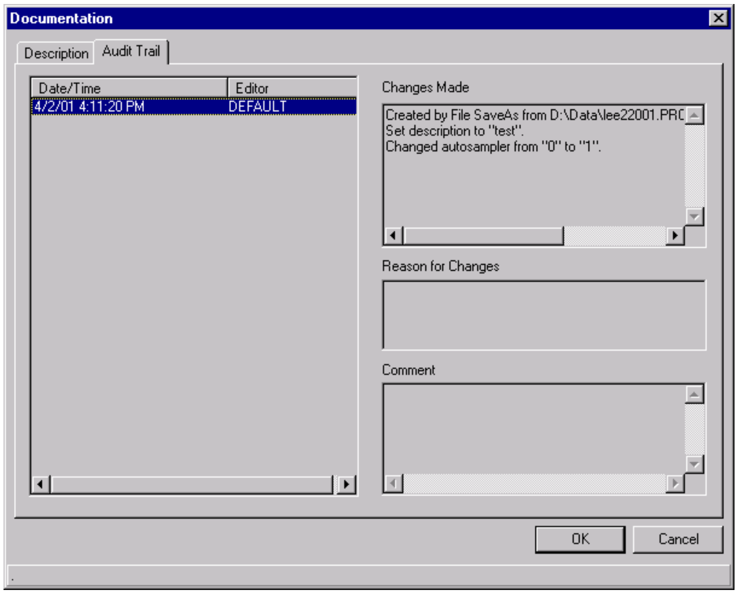
The **Description** tab opens when you save a new file, and (if auditing is not enabled) when you select **Save As** to save an existing file with a new name. You can also select **Description** from the **File** menu to open the Documentation dialog showing the **Description** tab.

Entering information in the Description tab

1. Enter any descriptive information about the file that you want to store with it. To start a new line, press CTRL+M.



2. If you want to start tracking changes to the file, select **Start audit trail**.



This will cause the Audit Trail dialog to appear every time you save this file in the future.

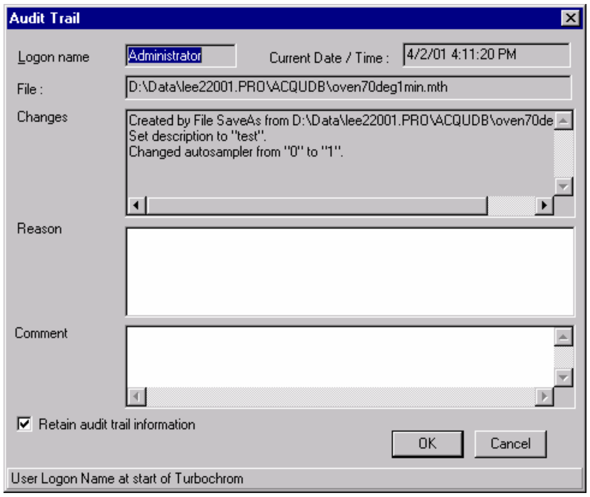
3. Click **OK**.

Audit Trail Dialog

If you previously enabled auditing for a file, the Audit Trail dialog appears every time you save the file or select **Save As** to save it under a new name. This dialog cannot be opened manually by any menu command or button.

Entering information in the Audit Trail dialog

1. Select a reason for the change(s) in the Reason field.



2. Enter any information about the change(s) you made to the file in the **Comment** field.

3. If you are saving the existing file as a new file (Save As), select **Retain Audit Trail Information** if you want to copy the Audit Trail information from the existing file to the new file and have auditing enabled in the new file.

4. Click **OK**.

   The information you enter in the Audit Trail dialog is saved with the file that you are auditing.

The Audit Trail

The Audit Trail tab in the Documentation dialog displays a history of changes made to the audited file. It appears when you select **Display Audit Trail** from the **File** menu. You cannot edit the information in this tab.

Viewing the Audit Trail

1. Select **Display Audit Trail** from the **File** menu.

2. When you have finished viewing the information, click **OK**.

Printing the Audit Trail

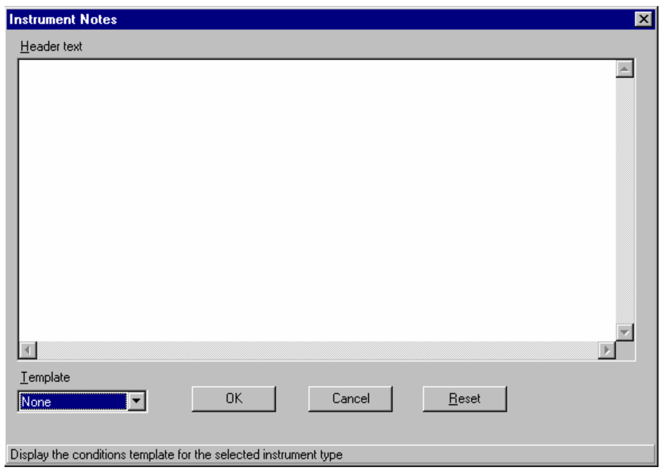
TurboMass displays a print options dialog when you select **Print** from the Method Editor **File** menu. This dialog includes an option to print the Audit Trail for the current file.

Creating Instrument Notes

The **Notes** command in the **Instrument** menu lets you create original text or use the preset template to record information about the instrument section of the method. The information you enter has no effect on data analysis. You can view these notes when you select **Print Preview** from the Method Editor **File** menu. You can print these notes when you print the full method.

Creating or editing header information for the GC method

1. Select **Notes** from the **Instrument** menu to open the Instrument Notes dialog.



2. Enter the header text that you want to appear in the printed reports for this method. To start a new line, press CTRL+M. To erase the contents of the text field, click **Reset**.

OR

Select the **CAP-GC** template from the **Template** drop-down list.

3. If you are working with the CAP-GC template, edit the information as necessary.

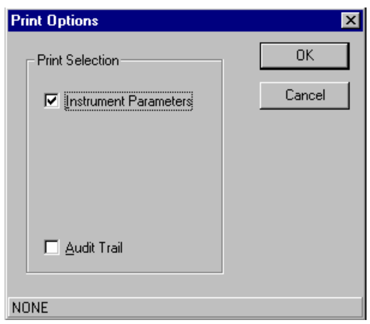
4. Click **OK** to save your changes.

Printing GC Method Parameters

You can print either the specific parameters from a GC method file or the summary information for a method by using the **File** menu **Print** or **Print Summary** commands. Two print-related dialogs will appear when you print parameters: one for method editor options and one for standard printing options.

Printing the parameters from the method

1. Select **Print** from the **File** menu to open the Print Options dialog.



2. Select the data to print and click **OK**.

3. Make any changes in the Print dialog, and click **OK**.

Printing summary information for a method

1. Select **Print Summary** from the **File** menu to open the Print dialog.

2. Make any changes in the Print dialog, and click **OK**.

Controlling the GC

Some GC-related menu choices are commands that let you control the GC:

- Equilibrate.
- Stop GC and Retry Injection.
- Take and Release Control.

Equilibrating the GC

GC Equilibration sends the GC method temperature and pressure settings to the GC to enable the GC to reach those setpoints in preparation for sample injection and data acquisition.

Equilibrating the GC

Select **Equilibrate** from the **Method Editor** menu.

The mass spectrometry sends the GC method temperature and pressure settings to the GC and begins equilibration.

The GC status in the top level window indicates that MS is equilibrating the GC.

When equilibration is complete, the GC status changes to Ready.

Stopping and Restarting the GC

If there is a problem with the GC setup after a run is started, the **Stop** command lets you stop the analysis. Once you have corrected the problem, **Retry Injection** lets you restart the GC without stopping and restarting your mass spectrometer method.

NOTE: *Stopping the GC from the* **GC** *menu does not stop MS data acquisition.*

Selecting **Stop** from the **GC** menu stops the method that is in the inlet file cell of the Sample List; however, the mass spectrometer is still acquiring data.

To stop MS data acquisition, select **Stop** from the TurboMass top level window **Run** menu, and respond whether you want to stop the GC as well.

If you started the MS data acquisition from the Tune page **Window** menu, stop the MS data acquisition, and select **Stop GC** from the Configuration Editor **GC** menu if you want to stop the GC also.

Releasing and Taking Control of the GC

The **Release** command lets you release the GC from mass spectrometer control to change a setting from the GC keypad or to make a hardware change to the GC. Once you have completed your change(s), you must re-establish (Take) control of the GC.

Releasing control of the GC

- From the **GC** menu, select **Release Control**.

  The **Take Control** command in the **GC** menu allows you to take control of the GC if its current GC status is Released. Usually, you do not have to select **Take Control** because this occurs automatically when you start your MS data acquisition. However, you may need to select **Take Control** if you previously selected **Release Control**.

Taking control of the GC

- From the **GC** menu, select **Take Control**.

The Details Window

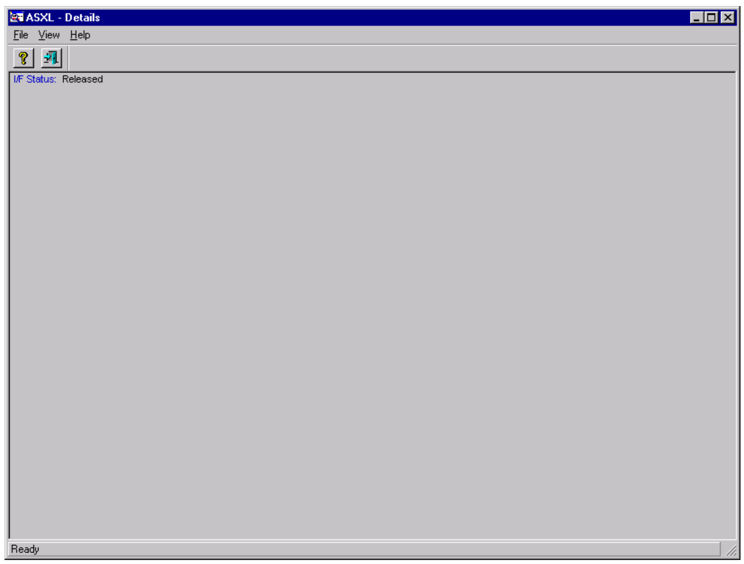
The **Details** command lets you see the GC run and interface status information.

The specific contents of the Details window depend upon whether you are collecting data from a Clarus detector.

Text appearing in blue on your screen represents information that is changing dynamically as the GC status changes. Text appearing in gray represents information that does not apply to this setup.

Viewing detailed status and run information

➢ Select **Details** from the **GC** menu to open the Details window.



Viewing a Real-Time Plot of GC Detector Data

You can view a real-time plot of GC detector data, for example a plot from a flame ionization detector (FID).

To display the real-time plot:

- Select **Real-Time Plot** from the **GC** menu.

NOTE: *The GC method file must be available in order for the software to display the real-time plot.*

Viewing Data Acquisition Information

The information that appears in the Details window is grouped into several categories.

Sample Information

Vial Number	Number of the sample as specified in the Sample List.
Raw Data File Ch A (Ch B, or both)	The full name of the current raw data file (for each active channel). This information appears only if data are being saved from a Clarus detector.

Analysis Information

Instrument Method	The name of the current method used for instrument control.
Run Time	The total length of time the current cycle is to run.
Delay Time	The amount of time between the start of the run and when data will be analyzed.
Sampling Rate	The number of data points acquired per second.

Viewing Detailed Instrument Information

The Details window displays information about the state of the GC.

Current

This section summarizes some of the more important current values.

I/F Status Status of the interface. For more information, refer to *Understanding GC Status Messages* on page 185.

Elapsed Time The amount of time, in minutes, that the current cycle has been running.

Aux Current flow/pressure.

Carr A/B Current carrier flow/pressure

Inj. A/B Current injector temperature.

Oven Temp Current oven temperature.

Program Time Length of time to run the oven program.

Zones

The setpoint (**Init Set**) for all zones might change during a run if you have set any timed events. The column will indicate **Ready**, **Not Ready**, **Alarm**, or **N/A**.

Injector Temp

Init Set Setpoint temperatures for injectors A and B.

Actual Current (actual) temperatures of injectors A and B.

Ready Whether or not the injector is ready.

Detector Temp

Init Set Setpoint temperatures for detectors A and B.

Actual Current temperatures of detectors A and B.

Ready Whether or not the temperature zone is ready.

Carrier Pressure/Flow

Init Set The initial carrier setpoint for channels A and B.

Actual The current (actual) carrier pressure/flow of channels A and B.

Units Units configured for the carrier.

Ready Whether or not the carrier zone is ready.

Detector Flow

Init Set The setpoint detector flow (two flows can be associated with each injector).

Actual The current (actual) detector flow of detectors A and B.

Ready Whether or not the detector flow zone is ready.

Auxiliary Pressure/Flow

Init Set The initial setpoint pressure/flow for auxiliary zones 1 through 4. The actual value might differ from the Init value due to timed events.

Actual The current (actual) pressure/flow of auxiliary zones 1 through 4.

Units Units configured for the carrier.

Ready Whether or not the pressure/flow is ready for the auxiliary zones.

Split Flow

Init Set The setpoint displayed as either flow or ratio depending on which mode you are using. The actual value might differ from the Init value due to timed events.

Actual The current (actual) flow.

Ready Whether or not the split flow zone is ready.

Understanding GC Status Messages

The status is displayed in the top level TurboMass window in the GC Status area. The status area displays the general status, the GC status, and the oven status.

The status information changes constantly as you acquire data, modify GC methods, and perform other actions that affect the GC.

NOTE: *The GC status must be either "No Method" or "Run Done" to successfully set up. Otherwise GC communication lockups may occur.*

The General and GC Status messages are color coded as follows:

Green Indicates that the instrument is ready to start a run (acquire data).

Blue Indicates that the interface is active (a run is in progress, or the interface is uploading data to TurboMass).

Red Shows that the instrument is not ready to collect data because it is not connected, it has no method, or it has been paused.

General Status

Active The interface is collecting data from a current GC run.

Backlog Data from one or more completed runs still reside in the interface.

Detached Not currently communicating with the interface, possibly due to communication errors.

Not Connected The instrument is not turned on or it is not connected to the

computer.

Init Error An error occurred during initialization.

Initializing TurboMass is retrieving initial status information for the interface.

In Reconfig The interface is reconfiguring itself, for example, updating the IPM.

No Method The interface is turned on and connected to computer but is not set up, or there is no method downloaded.

Post-Run Post-run activity is in progress or the autosampler is cleaning up after the previous injection.

Pre-Run The autosampler is preparing the next injection.

Ready The interface is ready to collect data and is waiting for the run to start.

Run Done The run is complete. The instrument must be initialized again for any future analyses.

Run Log The GC is uploading Run Log information to TurboMass.

Setting Up The instrument is being initialized with acquisition information.

System Reconfig TurboMass is carrying out a system reconfiguration.

GC Status

Equil The GC is equilibrating.

Hold The GC temperature program is in a hold state.

Not Ready	The GC is not ready.
Off	The GC is turned off.
Oven Off	The GC oven is turned off.
Pre-Run	The GC is executing the pre-run events.
Ready	The GC is ready.
PPC Alarm	The PPC pneumatics are in a fault condition.

During the oven temperature program, the current program step appears. These are: Initial (temp), Ramp 1, Hold 1, Ramp 2, Hold 2, Ramp 3, Hold 3, and Cool.

Oven Temperature

Oven temperature is displayed as an integer and may range from -99 to 450.

Viewing Error Messages

When an error occurs during configuration, method setup, or during a run, TurboMass displays an error message and saves it in the Error Log.

1. Select **Error Messages** from the **GC** menu to open the Error Log.
2. To print the Error Log, click **Print**.
3. To clear the Error Log, click **Clear**.

Working with the GC Interactively

There are two commands that let your work with the GC interactively, **Hands On** and **Modify Active**. **Hands On** lets you change some settings after GC setup. **Modify Active** lets you change a downloaded method.

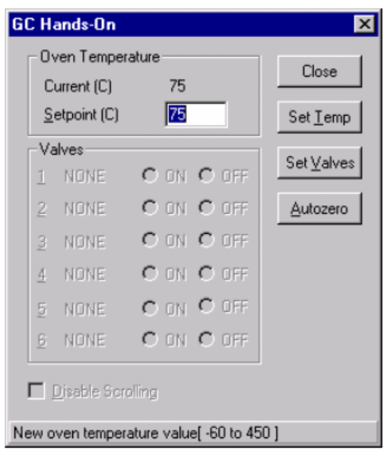
Using Hands On

The **Hands On** command in the **GC** menu lets you control certain settings after you have set up the GC. You can set the GC oven temperature, autozero the detector, and turn valves (or relays) on and off. You can access Hands On either during or outside of a run. The actual parameters available depend on whether or not a run is in progress. The Hands On command is not available until you have initialized the GC with a method.

Setting controls for the GC

1. Select **Hands On** from the **GC** menu, and click **Close**.

   The GC Hands On dialog is displayed, showing the oven temperature and the current valve settings.



2. In the **Setpoint** field, enter the setpoint oven temperature for the GC, and click **Set Temp**.

3. Click **Autozero**, if desired.

4. Select the valves you want to switch by selecting the **ON** or **OFF** button as appropriate.

5. Click **Set Valves** to implement the settings, and click **Close**.

   You must clickt **Set Temp**, **Set Valves**, or **Autozero** before clicking **Close** in order to change settings.

Modifying the Active Method

The **Modify Active** command in the **GC** menu lets you change method parameters in a method that has been downloaded by selecting **Start** from the TurboMass top level window **Run** menu.

When a method has been downloaded, it is by definition the active method — the one that is being used in the current run — and the Method Editor opens when you select the **Modify Active** command.

The commands and options available in the Method Editor depend on whether or not a run is in progress. When you modify the active method, the term Modify Active is displayed in the title bar of the Method Editor.

When you modify the active method with a run in progress, the instrument parameters that you can modify are limited to those that can be downloaded during a run. That is, you can modify the oven/inlet and detector parameters.

When you modify the active method and there is no run in progress, you can modify all method parameters in the active method.

When you finish editing the method, TurboMass downloads the modified method to the LINK and uses it for the next run.

NOTE: *If you select a method that is not the active method, you can modify all parameters within that method during or outside of a run.*

Modifying the downloaded method

1. Select **Modify Active** from the **GC** menu, or double-click the GC portion of the system icon in the Acquisition Control Panel

   OR

   Right-click the active method in the Inlet File cell in the Sample List.

   The GC method in use appears in the Modify Active (Method Editor) window.

2. In the Modify Active window, select a command from the **Instrument** menu to modify the parameters associated with that command.

3. Save your changes after editing method parameters.

   Note that the **Save As** command is not available because you cannot save the changes as a new method.

4. Close the Modify Active window.

   The GC Status field will display different messages, based on the instrument you are using. While you are modifying the method, the instrument state will be **Paused**. It will change to **Resumed** when you close the Modify Active window.

Function List Editor 8

Introduction

The Function List Editor is used to set up the function(s) that the mass spectrometer will use to scan the instrument during an acquisition. A function list can be a mixture of different scanning techniques that can be arranged to run either sequentially or concurrently during an acquisition. Typical uses for mixed function acquisitions are to acquire different SIR groups over different retention windows and the ability to switch MS scan mass ranges during an acquisition.

A function list is produced, saved on disk and then referenced by name when you start an acquisition.

The simple function list shown might contain only one function, for example, a centroided mode full scan between 50 and 550 amu using EI ionization. Immediately above the function bar display is a time scale that shows when the function will be active from and for how long it will run. In this case the function starts after 5 minutes and then runs for 35 minutes, terminating after a total elapsed time of 40 minutes.

➢ To open this dialog, open the MS Method from the Sample list

OR

Click  in the MS panel in the TurboMass main window.

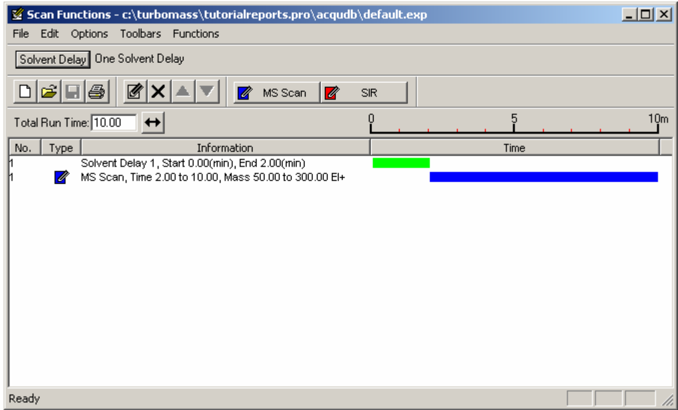


Figure 7 Function list showing a single function

The currently selected function is highlighted. If the display shows more than one function, you can select a new function either by selecting it, or by moving to it using the up or down arrow keys on the keyboard.

A more complicated function list might have four SIR functions, running sequentially for 10 minutes each.

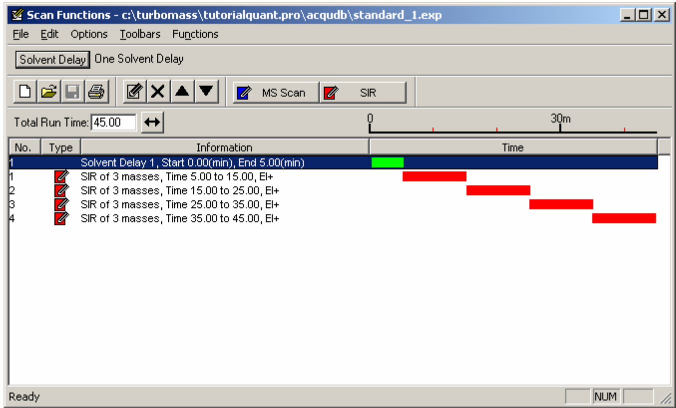


Figure 8 Function List showing multi functions

Up to 32 functions may be created in the function list.

A more advanced technique, Selected Ion and Full Ion Scanning (SIFI) has a mix of MS scan and SIR functions. As an example, it may have a single full MS scan method that runs for the entire chromatogram and multiple SIR functions timed for the elution of specific compounds. This allows both the universality of full scan analysis, with the ability to library search, and the higher sensitivity of SIR.

Function List Editor

Adding a New Function

A new function can be added either by clicking one of the function buttons at the top of the editor, or by selecting **MS Scan or SIR** from the **Functions** menu. The editor for the function type selected will be displayed showing default values. Make any changes required to the parameters and click **OK** to add the new function.

Modifying an Existing Function

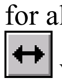
An existing function can be modified by double-clicking on the function in the function list. This will bring up the appropriate editor for the function type and allow you to change the function information. When you have finished editing the function, the function list display will be updated to show any changes.

Removing a Function

You can remove a function by selecting it and then selecting **Delete** from the **Edit** menu.

Changing a Function's Start and End Times

You can change the start and end times of a function by going into its editor as described in *Modifying an Existing Function* on page 196.

The **Total Run Time** field in the Scan Functions window shows the total run time for all the functions. Entering a new value in the **Total Run Time** field and clicking  will set the maximum retention time for the experiment. The ratio of the functions defined will be maintained. For example, if two functions are defined one from 0 to 5 minutes and the other 5 to 10 minutes then a **Total Run Time** of 10 minutes will be displayed. If this value is changed to 20 (and  is clicked) then the first function will now run from 0 to 10 minutes and the second from 10 to 20 minutes.

Setting a Solvent Delay

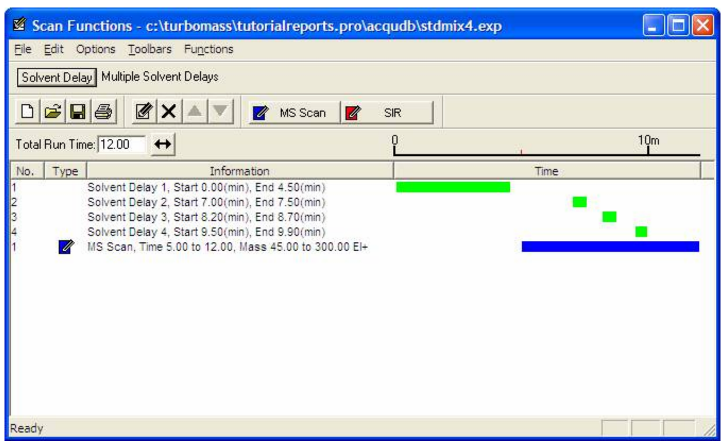
A solvent delay can be set for a function list using the Solvent Delay Time control. No data is stored during the solvent delay period, which means that solvent peaks that would normally be seen eluting at this time on the TIC chromatogram of the acquired data will no longer be seen. The filament in the source is turned off during the solvent delay to prevent it from being damaged.

The <Enter> or arrow key must be pressed after changing the solvent delay.

Multiple Solvent Delays

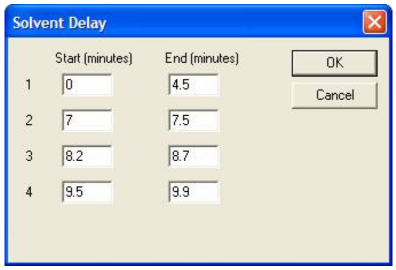
There are instances where a chromatogram has several peaks large enough that you would want to turn off the filament while they are eluting to protect the filament from burn-out, and then turn it back on afterwards and continue the analysis. The multiple solvent delay functionality is designed to accommodate this along with the conventional solvent delay at the beginning of the chromatographic run.

The MS Method editor has a “Solvent Delay” button. When selected, it brings up a dialog allowing up to four solvent delays to be specified.



Solvent delays are displayed in the method bar as bright green bars at the top of the Function display, and numbered from 1 to 4. Double clicking on a solvent delay bar, or clicking the edit button with a solvent delay selected, brings up the solvent delay dialog. Pressing the “X” delete button or pressing the delete key with a solvent delay

selected will remove a solvent delay. If it is between other delays, then the delays are shuffled up.



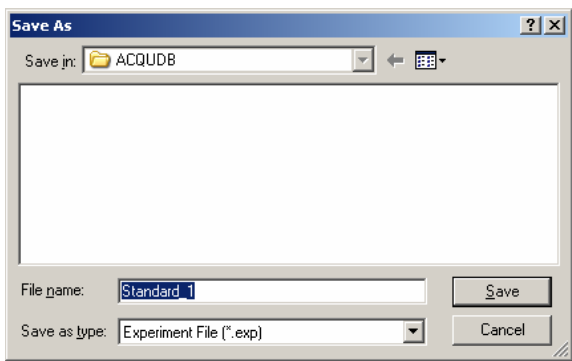
If just one conventional solvent delay is used, only the top "End" box should be filled in, with all the other values set to 0. Solvent delays may not overlap, and must be entered in order of increasing retention time.

Saving and Restoring an MS Method

Saving an MS Method

1. Select **Save As** from the MS Method **File** menu to display the Save File As dialog.

2. Enter a new File Name under which you want the MS Method to be saved, or select an existing file from the list displayed.

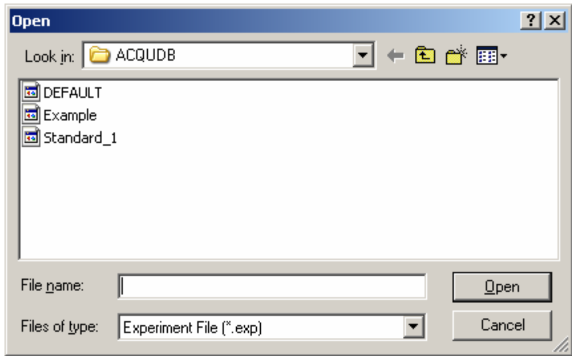


3. Click **Save**.

If the selected file already exists, you will be asked to confirm that you want to overwrite the existing information. Click **Save** to continue, or **Cancel** and specify a different name.

Restoring a saved MS Method

1. Select **Open** from the MS Method **File** menu to display the Open dialog.



2. Select the File Name of the MS Method that you would like to use, either by entering its name or by selecting it from the displayed list, and click **Open**.

   OR

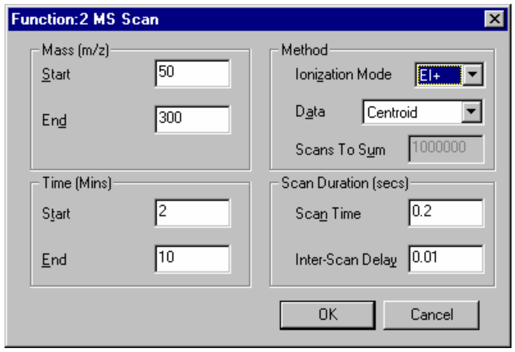
   Right-click on the desired MS Method in the Sample List and click **Open**.

Setting Up an MS Scan Function

The MS scan function editor is used to set up centroid, continuum and MCA functions.

1. Click **MS Scan** to open the MS Scan Function Editor.

2. Enter the scan function parameters.



Start Mass Specifies the mass at which the scan will start. The Start Mass must be lower than the End Mass.

End Mass Specifies the mass at which the scan will stop. Both the start and end masses can be selected directly from a spectrum displayed in the Spectrum window. If you right-click and drag the mouse across a spectrum, TurboMass will automatically enter the start and end mass values for the selected mass range.

Ionization Mode Specifies the ionization mode and polarity that will be used during the acquisition.

WARNING

Do not select **EI+** *if a CI ion source is installed. The filament will not regulate properly.*

Data Specifies the type of data to be collected and stored on disk:

Centroid — Stores data as centroided, intensity, and mass assigned peaks. Data are stored for every scan. Almost always used for GC/MS.

Continuum — Data are not centroided into peaks. Instead the

signal received by the interface electronics is stored regularly to give an analog intensity picture of the data being acquired. Data are stored for every scan.

As data is being acquired and continuously stored to disk, even when there are no peaks being acquired, continuum data acquisition places some extra burden on the acquisition system as compared to centroided acquisition. Data file sizes will tend to be significantly larger than centroided one sided, and the absolute scanning speed (Da/sec) will be slower. You can set a threshold below which the data will not be stored to disk, which can reduce these effects, depending on the nature of the data being acquired.

You can set the threshold so that data considered to be “noise” can be discarded, thereby improving data acquisition speed and reducing data file sizes. For more information about setting instrument data thresholds, see *Setting Instrument Data Thresholds* on page 70.

Multi Channel Analysis (MCA) — MCA data can be thought of as “summed continuum” with only one intensity accumulated scan being stored to disk for a given experiment. As each scan is acquired, its intensity data is added to the accumulated summed data of previous scans. An advantage of MCA is that random noise will not accumulate as rapidly as real data and, therefore will effectively average out over a number of scans. This will emphasize the real data and improve the signal-to-noise ratio. A further advantage of MCA is that as data is written to disk only at the end of an experiment, scanning speeds can be increased and significantly less storage space is required. The disadvantage of MCA is that as there is only one scan, it cannot be used for time resolved data.

Scans To Sum For MCA scans, this defines the number of scans to sum to create a spectrum.

Start Time Specifies the retention time in minutes at which this function will become active; that is, data acquired and stored.

End Time Specifies the retention time in minutes at which this function will cease to be active; that is, data acquired and stored.

Scan Time Specifies the duration of each scan in seconds.

Inter-Scan Delay Specifies the time in seconds between a scan finishing and the next one starting. During this period data is stored, but not acquired.

The total time for a scan = Scan Time + Inter-Scan Delay.

Scan rate = (Start Mass – End Mass) / Scan Time (Da/sec)

Scans/sec = 1 / Scan Time + Inter-Scan time

Setting Up an SIR Function

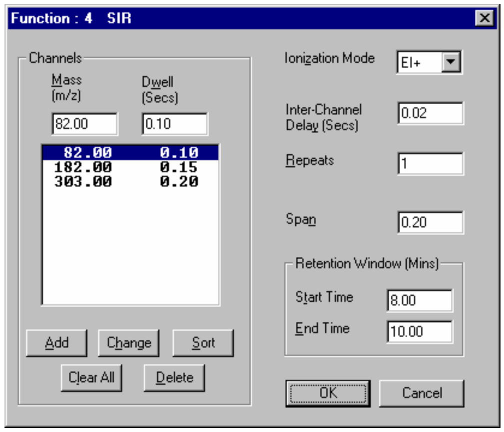
The SIR (Selected Ion Recording) technique is typically used in those situations where only a few specific masses are to be monitored during an acquisition. Since most of the data acquisition time is spent on these masses, the SIR technique is far more sensitive than "full scanning." The signal-to-noise ratio increases with the square root of the dwell time.

The SIR editor is used to enter the masses that you would like to monitor, and their respective dwell time, span and inter-channel delay time.

When possible we try to monitor ions characteristic of the compound, as high in mass and intensity as possible. High mass is desirable to minimize the probability of chemical interference (selectivity). High intensity is desirable for sensitivity. We also try to choose ions with low baselines for these same reasons.

1. Click **SIR** in the Scan Functions dialog.

   The SIR dialog is displayed.



1. Specify your parameters.

   Most of the parameters are the same as those in the MS Scan Editor. However, the following are different:

Mass Specifies the mass to be monitored up to a maximum of 32. A mass can be entered either by entering its value into the Mass field and pressing ENTER or by clicking **Add**. The mass can be calculated if the chemical formula of the ion is known with the **MW Calculator** function in the top level **Tools** menu. The mass may also be pulled directly from a spectrum displayed in the Spectrum window. To do this, display the required spectrum in the Spectrum window, and right-click the ions that you wish to monitor. As you select a mass, it will appear in the SIR masses table.

Dwell Specifies the length of time in seconds for which the highlighted mass will be monitored. This is normally set so that the sum of all the **Dwell** times for all the target ions gives about 10 scans across the GC peaks.

Inter Channel Delay Specifies the length of time in seconds between finishing monitoring the highlighted mass and starting monitoring the next mass in the function.

Repeats This is only relevant for experiments having more than one function and specifies the number of times we wish to execute this Function per pass. For example, if we had two Functions defined by their Start Time and End Time to execute simultaneously, and the first Function has Repeats = 1, while the second has Repeats = 3, then the second Function would execute three times for each time the first Function executed once. With non-overlapped Functions, better detection limits will be obtained by increasing the **Dwell** time rather than the number of **Repeats**.

Span Specifies a small mass window applied centrally about the highlighted mass. During acquisition this range will be scanned over the specified **Dwell** time. This minimizes the chance of missing the top of the mass peak. A span of zero can be set to simply "sit" on the specified mass for maximum sensitivity.

Add Enter values into the **Mass** and **Dwell** fields and then click **Add** to add the new Mass to the list.

Change Left-click on a mass in the list and then click **Change** to change the **Mass** or **Dwell**.

Sort Sorts the list in order of ascending Mass.

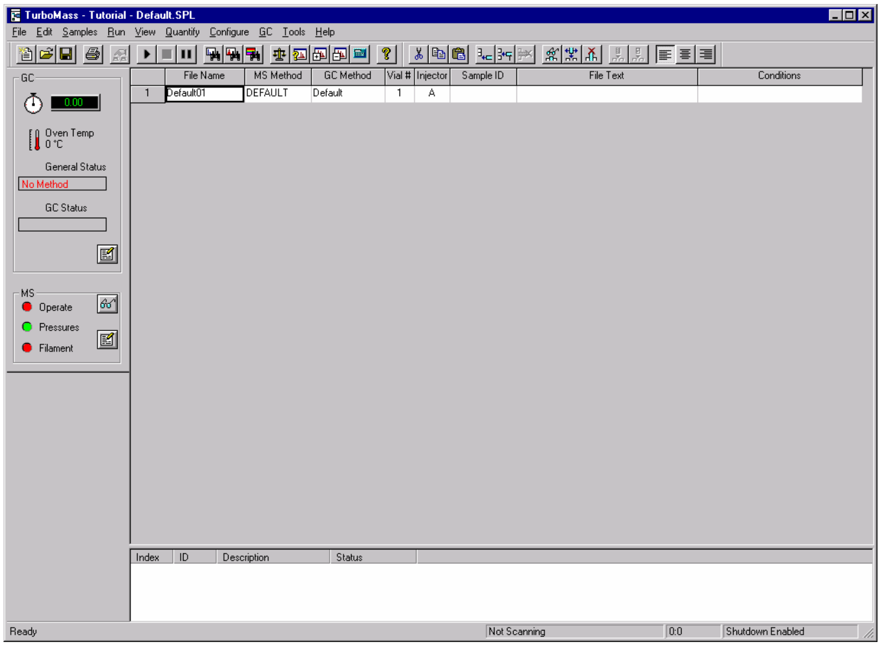
Clear All Deletes the list of Masses.

Delete Left-click a mass in the list and then click **Delete** to delete a single Mass.

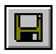
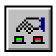
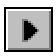
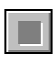
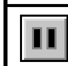
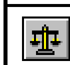
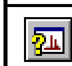
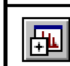
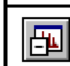
Sample List 9

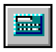
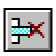
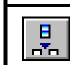
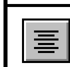
Top Level Menu

The top level desktop includes menus and toolbar buttons that allow you to create and modify Sample Lists.



The TurboMass Menu Toolbar

Button	Menu Equivalent	Purpose
	File… New	Create a new Sample List
	File… Open	Open an existing Sample List
	File… Save, or File… Save As	Save a Sample List
	File… Print	Print a Sample List
	Run… Control Panel	Only applicable to previous versions of software
	Run… Start	Start an acquisition
	Run… Stop	Stop an acquisition
	Run… Pause Queue	Pause the queue of acquisitions
	View… Spectrum	View Spectrum
	View… Chromatogram	View Chromatogram
	View… Map	View Map
	Quantify… View Results	View Quantify Results
	Tools… Search Library	Perform a Library search
	Tools… Combine Functions	Combine Functions
	Tools… Strip	Strip Functions

Button	Menu Equivalent	Purpose
	Tools… MW Calculator	Invoke Molecular Weight Calculator
	Help… About TurboMass	Display program information, version number and copyright
	Edit… Cut	Cut the selection and put it on the clipboard
	Edit… Copy	Copy the selection and put it on the clipboard
	Edit… Paste	Paste the contents of the clipboard
	Samples… Add	Add samples to the Sample List
	Samples… Insert	Insert samples into the Sample List
	Samples… Delete	Delete samples from the Sample List
	Samples… Field… Properties	Invoke the Field Properties dialog
	Samples… Field… Customize Display	Invoke the Customize Field Display dialog
	Samples… Field… Remove Column	Remove a field from the display
	Samples… Fill… Down	Fill down
	Samples… Fill… Series	Fill series
	Samples… Field… Align… Left	Align text to the left in the current column
	Samples… Field… Align… Center	Align text to the center of the current column

Button	Menu Equivalent	Purpose
	Samples… Field… Align… Right	Align text to the right in the current column
	Samples…Sample List Wizard	Invokes the Sample List Wizard
The following icons are shown in the TurboMass GC and MS panels		
		Opens the GC Method Editor
		Opens the Tune window
		Opens the MS method

Creating and Editing Sample Lists

NOTE: *The Sample List is saved with the .RAW data file when data is acquired. If you change the Sample ID field in the sample list and try to print environmental reports, the Sample ID reverts back to the original setting when the files were acquired. You may want to change the Sample ID field if you modify the sample list to acquire new samples.*

Creating a new Sample List

To create a new Sample List:

1. Click 

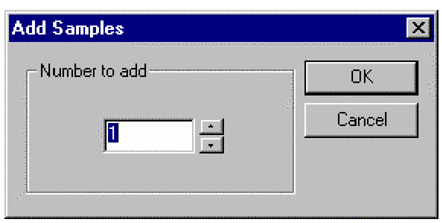
   OR

   Select **New** from the **File** menu to display a Sample List with one default row displayed.

   OR

   Create a Sample List using the Sample List Wizard (See the Sample List Wizard on page

2. Add the desired number of rows to the Sample List by either clicking **Add Row**  to display the Add Samples dialog, editing the **Number to add**, and clicking **OK**.

   OR

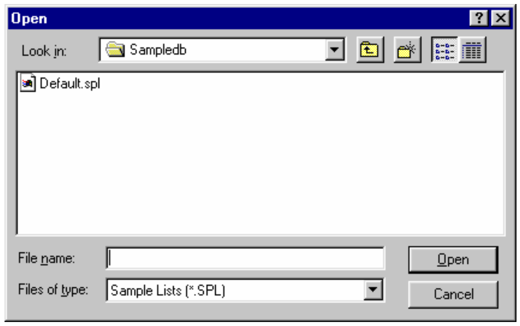
   Selecting the desired number of rows in the Sample List, and clicking **Insert**.

Opening an existing Sample List

1. Click 

   OR

   Select **Open** from the **File** menu to display the Open file dialog.



2. Select a data file and click **Open**.

Creating a Sample List Using the Sample List Wizard

The TurboMass Sample List window is in a spreadsheet format, which allows easy editing of multiple samples but this becomes unwieldy when there is a lot of information required for each sample. The Sample List Wizard is a forms-format equivalent display. It allows for easier editing of the large amount of per-sample information required of environmental and QA/QC samples.

The Sample List Wizard enables you to select an existing sample list or create a new one. Only the parameters required for the current type of analysis (VOA, SV, or QA/QC) and current matrix (water/soil) are displayed. The controls are grouped in a way to allow efficient entry of sample-specific data. It also provides the ability to propagate changes made to one row to subsequent rows; a command to update vial numbers; a command to update sample IDs. Several fields have automatic incrementing of numeric values, and there are commands to insert, delete, and add sample rows.

NOTE: All environmental reporting users should use the Sample List Wizard to ensure that all sample information is entered.

You can enter or modify all of your environmental and QA/QC sample list parameters using the Sample List Wizard. You can still edit directly from the Sample List.

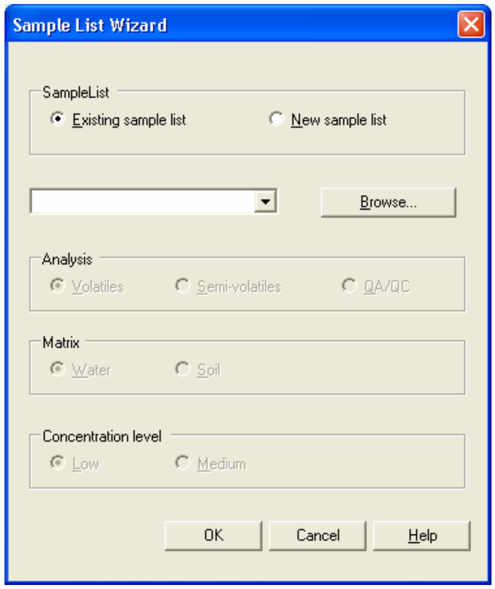
The recommended approach to using the Sample List Wizard is to create your original "template" sample list so that all the per-sample information is correctly filled in. When you run later sets of samples which follow a similar sequence you may then read in the original "template" sample list, rename it, and make your per-sample changes in the Wizard or sample list window spreadsheet environment – which ever you find most convenient for your current task.

More specifically the Sample List Wizard provides:

- The ability to read an existing sample list template.
- Only the parameters required for the current analysis (VOA, SV, or QA/QC) and current matrix (water/soil) are displayed.
- Grouping of controls for efficient entry of sample-specific data.
- The ability to propagate changes made in one row to subsequent rows.
- A command to update vial numbers.
- A command to update sample IDs with automatic incrementing of numeric values.

Setting Up the Sample List Wizard

The *Sample List Wizard dialog* (started from the Samples/Sample List Wizard dialog) provides you with the ability to select and specify an **existing sample list** or create a **new sample list**. The display of editable sample parameters will depend on your choice of Analysis, Matrix, and Concentration Level.



The parameters required for the current **analysis** (VOA, SV, or QA/QC) and current **matrix** (water/soil) are displayed. The controls are grouped in a way to allow efficient entry of sample-specific data. It also provides the ability to propagate changes made to one row to subsequent rows; a command to update vial numbers; and a command to update sample IDs, including automatic incrementing of a numeric value. The parameters are:

- Sample List
- Analysis
- Matrix
- Concentration Level

NOTE: *When you select an existing sample list, the controls in the Analysis. Matrix and Levels section are disabled and use the values in the last row of that sample list to indicate the nature of the sample list (assumes all rows use same Analysis, Matrix and Level settings). If there are no entries for those columns (for example, if it was created prior to version 5.1) then the Analysis option will be set to QA/QC (and hence the other options will show no selection).*

Sample List	The Sample List section of the dialog provides you with the options of either selecting a new sample list or editing an existing sample list.
Existing sample list	Select this radio button to edit an **Existing sample list** file. When selected, the <sample list file name> drop–down list and Browse button are enabled. All other controls in the dialog are be disabled (i.e., Analysis, Matrix and Level selections) as described above.
New sample list	Select this radio button to create a **New sample list**. When selected, the <sample list file name> drop–down list control and Browse button are disabled.
	Select a sample list in the current Project from this field by pressing the down-arrow icon or search for another sample list by using the Browse button. This field is blank when the New Sample List option is selected. Clicking the Browse button displays the standard File Open dialog so that you can search for a stored sample list. Typically sample lists are found in the SampleDB directory of your Project directory (*.PRO).
Analysis	The Analysis section of the dialog is enabled when the New sample list option is selected. There are three radio buttons for this section: Volatiles, Semi-volatiles, and QA/QC. Volatiles and Semi-volatiles are environmental sample types. If either one is selected, the Matrix and Concentration Levels sections remains enabled. If QA/QC is checked, the Matrix and Concentration level sections will be disabled.
Volatiles	Select this radio button to indicate that the new sample list will be used for volatile organics analysis (VOA).
Semi-volatiles	Select this radio button to indicate the new sample list will be used for semi-volatile (SV) organics analysis.
QA/QC	Select this radio button to indicate the new sample list will be used for general quality assurance or quality control (QA/QC)

analysis purposes.

Matrix	The **Matrix** section is only enabled when you select a Volatiles or Semi-volatiles Analysis. Other matrices can be analyzed, but may require the use of additional scaling factors, custom reporting templates, or external calculations.
Water	Select this radio button to indicate that the new sample list will be used for the analysis of water samples. This (together with the Analysis setting) determines the calculations Quantify will use to produce concentration results. If Water is checked, the Concentration level section will be disabled.
Soil	Select this radio button to indicate that the new sample list will be used for the analysis of soil (or sediment) samples. This (together with the Analysis and Concentration level settings) determines the calculations Quantify will use to produce concentration results.

Concentration Level	The Concentration level section is only enabled when you select a Volatiles or Semi-volatiles analysis and a Soil matrix. Different equations are used for each.
Low	Select this radio button to indicate that the expected concentration range of soil samples to be analyzed with the sample list.
Medium	Select this radio button to indicate that the expected concentration range of soil samples to be analyzed with the sample list.
OK	Clicking the OK button displays the Sample List Wizard main window.
Cancel	Clicking the Cancel button closes the dialog and returns you to the main Sample List window.
Help	Clicking this button displays the Help window for this dialog.

Building a Sample List

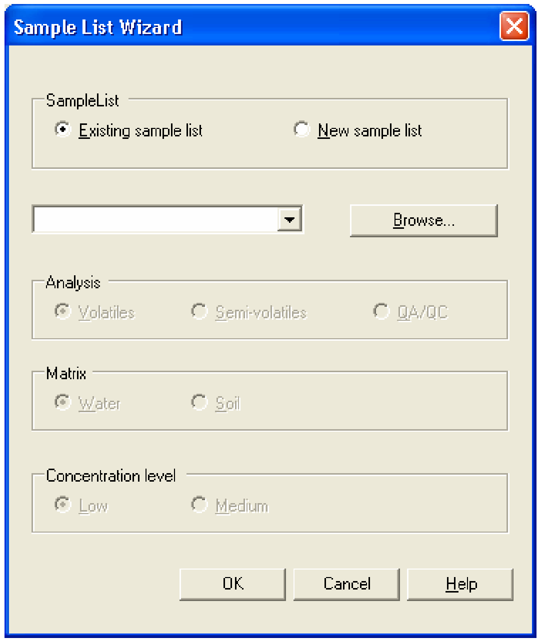
You can build a sample list manually or use the Sample List Wizard. This procedure describes how to use the Sample List Wizard to build your sample list.

In this example we will show how to use the Sample List Wizard to build a sample list.

1. Click 

   OR

   Select **Sample List Wizard** from the **File** menu to display the Sample List dialog.



You can modify an existing sample list or create a new sample list. This example shows how to build a new sample list.

2. Click the **New sample list** button.

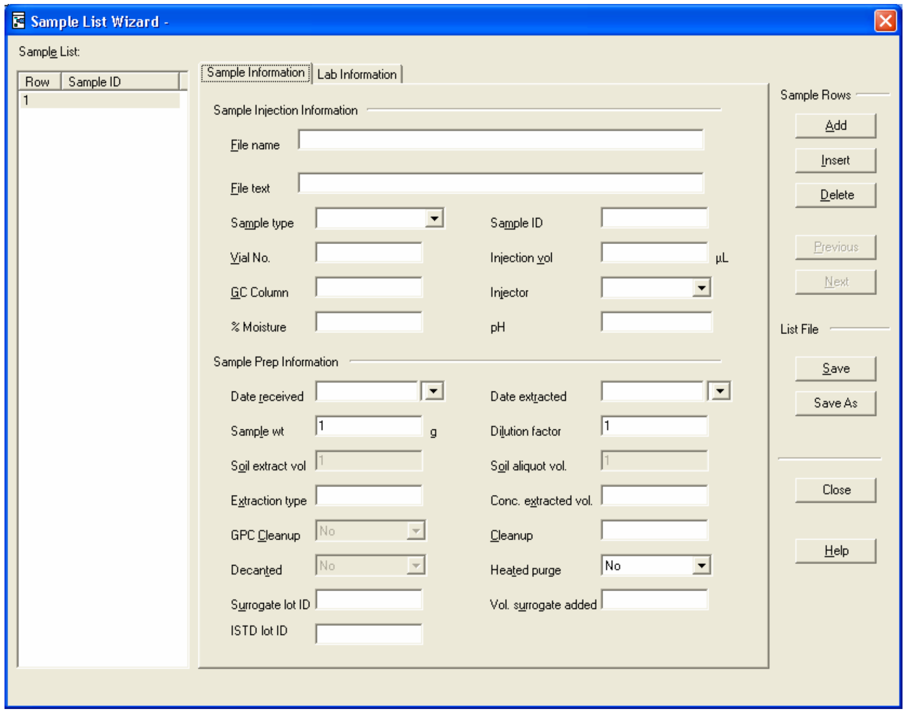
3. Select the type of **Analysis**. Volatiles, Semi-Volatiles or QA/QC

4. Select the **Matrix**. Soil or Water

5. Select a **Concentration level**, **Low** or **Medium**.

6. Click **OK**.

   The next dialog appears for you to enter the **Sample Information** and **Lab Information** for each of the Samples.



Adding Sample to the Sample List

The Sample List window is a listing of the **Row** numbers and **Sample ID**s for the samples in the current sample list. As long at least one sample exists in the list, a sample is always selected. The currently selected sample is indicated with a highlight. You can change the selected row using the up and down arrow keys or with the mouse. If the **Ctrl** key is held down, the up arrow will move the currently selected sample row up one position in the list. Similarly, with the Ctrl key held down, the down arrow will move the currently selected sample row down one position in the list.

- Enter the **Sample Injection** Information.
  This window contains many fields required for environmental and QA/QC data. Not all fields need to be entered since they are not used for calculations but only displayed on the reports. They can be ignored or added later on a LIMS system.

Sample Injection Information

File name - Enter the raw data file name.

File text - Enter additional comments about the sample.

Sample Type - Select the type of sample from a drop-down box. The following Sample Types are displayed in the order in which they are to appear in the drop–down list:

• Analyte	Analytical sample with unknown concentrations of target compounds.
• Analyte Dup	Reinjection of an Analyte.
• Blank	An analytical blank. For environmental and QA/QC, use Meth Blank instead.
• QC	Quality Control sample.
• Standard	Concentration calibration standard. For environmental and QA/QC, use Init Calib or Cont Calib instead.
• Tune Eval	DFTPP or BFB tuning check.
• Init Calib	Initial calibration standard (e.g. one level of a 5-level calibration).
• Cont Calib	Continuing Calibration standard (injected periodically to validate the initial calibration curve).
• Meth Blank	Analytical Method Blank. Contains all Internal Standards and Surrogates.
• Lab Control	Laboratory Control Sample (LCS), typically a Cont Calib prepared from a different stock solution to validate the Init Calib and Cont Calib concentrations.
• Spike	Matrix Spike sample.
• Spike Dup	Matrix Spike Duplicate sample.
• Dilution	Dilution of an Analyte. Sample List "Conc" values for internal standards and Surrogates will need to be adjusted if they are diluted.
• Re-Extract	Re-extracted sample.

Sample ID - Enter this primary sample descriptor for the environmental reporting software. This descriptor appears in the Sample List column in this window.

Vial No. - The sample position in the autosampler from which the injection will be made.

Injection vol - The amount of sample injected into the GC. **This value does not control the injection volume (that value is in the GC Method) but it is used in calculations.**

GC column - Enter information about the GC column used for the analysis. It is enabled if a GC is configured on the system.

Injector – Select from the drop-down list injection port (A or B) into which the sample will be injected (this controls the Clarus GC autosampler).

% Moisture - Enter the moisture content determined for a soil sample. This field is enabled only if the Matrix is Soil.

pH - Enter the pH of the sample.

Sample Prep Information

Date received - Date the sample was received in the lab. The date is displayed in the short format defined in the Windows Regional settings. Clicking the down arrow command button displays a calendar control, to enable you to select the Date received.

Dated extracted - Date the sample was extracted for analysis. The date will be displayed in the short format defined in the Windows Regional settings.

Clicking the down arrow command button displays a calendar control, to enable you to select the Date extracted.

Sample wt (Sample vol) - The weight or volume (depending on sample matrix) taken for analysis. This field is enabled if the Analysis type is Volatiles or Semi-volatiles.

> If the Matrix setting is Soil the caption is Sample wt and the units displayed are grams (g).
>
> If the Matrix setting is Water the caption is Sample vol the units displayed are milliters (mL).

Dilution factor - Dilution factor applied to the sample. (Undiluted is 1)

Soil extract vol - The total volume of the methanol extract. Enabled only if the Analysis type is Volatiles, the Matrix is Soil and the Concentration level is Medium.

Soil aliquot vol - Volume of the aliquot of the sample methanol extract. Enabled only if the Analysis type is Volatiles, the Matrix is Soil and the Concentration level is Medium.

Extraction type - A text field that indicates how the sample was extracted.

Conc. extract vol. - The concentrated extract volume. Enabled if the Analysis type is Volatiles or Semi-volatiles.

GPC Cleanup - A drop–down box that indicates whether or not the sample was subject to a GPC (gel permeation chromatography) cleanup procedure. Enabled if the Analysis type is Semi-volatiles.

Cleanup - A text field that describes any (non-GPC) cleanup procedure used. Enabled if the Analysis type is Volatiles or Semi-volatiles.

The following parameters are informational only used for reports

Decanted - A drop–down list that indicates whether or not the sample was decanted. Enabled only if the Analysis type is Semi-volatiles and Matrix is Soil.

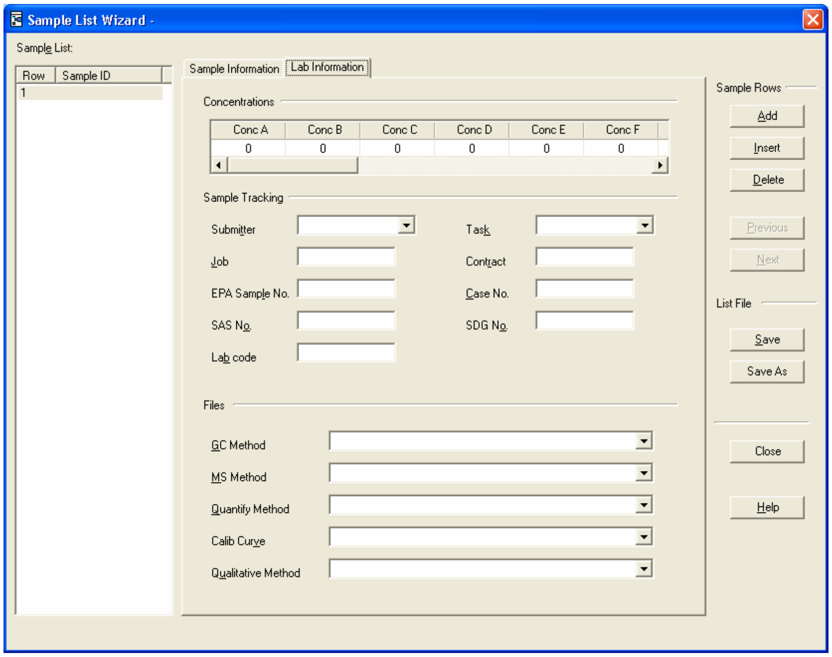
Heated purge - A drop–down box that indicates whether or not a heated purge was used. Enabled if the Analysis type is Volatiles or Semi-volatiles.

Surrogate lot ID. - A text field allowing identification of the lot number of the surrogate standard compounds mix. Enabled if the Analysis type is Volatiles or Semi-volatiles.

Vol surrogate added - An edit box that indicates the volume of surrogate standard added to the sample. This field is enabled if the Analysis type is Volatiles or Semi-volatiles.

ISTD lot no. - A text field allowing identification of the lot number of the internal standard compounds mix. Enabled if the Analysis type is Volatiles or Semi-volatiles. All concentration calculations for target compounds are made relative to an internal standard

- Click the Lab Information tab and enter the Lab Information for this sample. Lab information displays for each Sample ID in the Sample List. These values typically do not change on a per-sample basis, so they have been put in this second tab to simplify the user interface.



Concentrations Display – The concentrations grid (with a horizontal scroll bar) contains cells for you to enter standard Concentrations A to T (identical with the Conc A to T values shown in the sample list spreadsheet display). These concentrations levels are defined for the standard compounds in the Quantify method.

Sample Tracking

Submitter - Drop–down list of the Submitters previously entered in the Submitter/Task Data window.

Task - Drop–down list of the Tasks previously entered in Submitter/Task Data window. Optionally defines the list of compounds to be reported, reporting limits, and

printouts (report methods).

Job - Text field describing the job the sample is associated with.

Contract - Text field describing the contract under which the sample is being analyzed.

EPA sample No. - Text field defining the EPA sample number.

Case No. - Text field defining the case number.

SAS No. - Text field defining the Special Analytical Services (SAS) number.

SDG No. - Text field defining the Sample Delivery Group (SDG) number.

Lab Code - Text field containing the laboratory code.

Files

GC Method - A drop–down list enabling you to select the GC Method to be used for the analysis.

MS Method - A drop–down list enabling you to select the MS Method to be used for the analysis.

Quantify Method - A drop–down list enabling you to select the Quantify Method to be used for the analysis.

Calibration Curve - A drop–down list enabling you to select the calibration file to be used for the analysis.

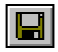
Qualitative Method - A drop–down list enabling you to select the Qualitative Method (typically the TIC library search) to be used for the analysis.

NOTE: *After editing a Sample List, the Environmental Reports generated do not reflect the Sample List until **Quantify is first run** on the new list.*

NOTE: *The Sample List is saved with the .RAW data file when data is acquired. If you change the Sample ID field in the Sample List and try to print Environmental Reports, the Sample ID reverts back to the original setting when the files were acquired. You may*

want to change the Sample ID field if you modify the Sample List to acquire new samples.

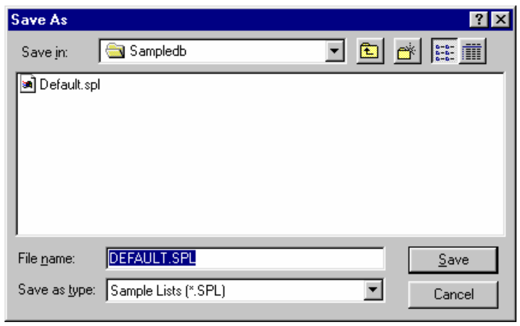
Saving a Sample List

1. Click 

   OR

   Select **Save** or **Save As** from the **File** menu.

   If this is a new Sample List, or the Save As option has been selected, the Save Sample List dialog is displayed.

2. Enter a name into the File Name field and click **Save**.

   The following characters cannot be used in the filename: / \ & . , : ? “ < >

Editing a Sample List by importing a worksheet from LIMS

The TurboMass software supports text file import for creating a Sample List from a LIMS worklist and text file export for passing results on to LIMS. The import file format is compatible with one generated by PerkinElmer LABWORKS™ but it can be generated by most LIMS systems. See Appendix E
LIMS Import File Example.

The imported file contains one line per sample list row and each line will consist of some or all of the (functional) parameters that can be defined in a row. The text file

contains a definition of which fields (columns) the text file is defining for each sample list row. The names used in this list will be the database field names for the columns. Text items that contain the defined separator character (e.g. commas) must be enclosed in quotes " ". If quotes are to be included in a string enclosed in quotes, they must appear twice (e.g. "This string contains not only a comma, but also ""quotes"" within it").

The import operation appends the sample rows defined in the text file to the currently displayed sample list. However, if the current sample list is 'blank' (following a File/New command) the imported sample list will overwrite the blank line and append subsequent lines. For the purpose of determining a 'blank' sample list, the fact that the File Name cell is empty will be sufficient.

To import a Sample List from LIMS:

NOTE: *The key thing to remember is that each Sample List file must have two sections: The [Variable Parameter List] and the [Variable Parameter Data]. The Number of Parameters in the [Variable Parameter List] must equal the number of values in the Data string. For example, if the NumberOfParameters=56 then there should be 56 entries after Data= .*

1. On the Sample List page, select **Import Worksheet** from the File menu.

   The Worksheet Names dialog appears.

2. Click the drop-down button next to Look in and search for the directory containing your files.

3. When you find your desired file, click open.

NOTE: *We have provided a sample worksheet for import (Templates_LIMS_import.txt) in the C:\TurboMass\TutorialReports.pro\SampleDB directory.*

NOTE: *If an error occurs during generation of the sample list, rows read from the text file that were valid will be added to the sample list and an error message will be displayed indicating the error. Further processing of the text file will stop at the occurrence of an error.*

Possible errors and the displayed messages include:

- First line of text file does not contain column names – “The first line of the import file must list the columns to be used”
- Invalid name included on first line – “The first line of the import file contains an invalid column name: <the invalid name>”
- Incorrect number of data items on a line – “Incorrect number of items on line: <line number>”
- Invalid data type – “Invalid data type on line <line number> : <column name> (<required data type>)”

Copying a spreadsheet into the Sample List

To copy a spreadsheet created in another application into the Sample List:

1. Click 

   OR

   Select **New** from the **File** menu to display a Sample List with one default row.

2. Add rows and columns to the Sample List so that it has the same number of rows and columns as the worksheet in the other Windows application.

NOTE: *If the number of rows and columns displayed in the Sample List is not the same as in the other Windows application, data may be lost.*

3. Select the relevant area in the other Windows application and copy it.

4. To modify currently displayed rows in the Sample List Editor, position the cursor on the cell at the top left corner of the paste area, and click **Paste**.

Printing a Sample List

1. Click 

   OR

   Select **Print** from the **File** menu to display the Print dialog.

2. Select the printer, print range, number of copies, and click **OK**.

Formatting Sample Lists

Column widths can be changed in the same way as any Windows spreadsheet.

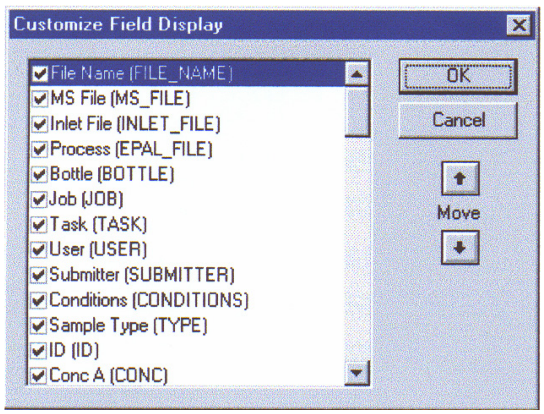
There are many different columns of information that can be displayed in the Sample List.

Selecting columns for display

1. Click 

   OR

   Select **Customize Display** from the Field option on the **Samples** menu to open the Customize Field Display dialog.



2. Select the appropriate checkboxes to include the appropriate fields (columns) in the Sample List. The following fields can be used for GC/MS.

File Name	The analog of MS data file name.
MS Method (MS_File)	The MS method file name.

GC Method (Inlet_File)	The GC method file name.
MS Tune File	The name of the file that contains the MS tuning parameters. If left blank, the current tune file settings are used.
Injector (Inlet_Switch)	Specifies the GC injector site used to introduce the sample. "A" is the front Clarus 500 GC injector and "B" is the rear.
Injection Volume	Not used for TurboMass control only for quantitative calculations.

NOTE: *The injection volume is set in the GC method.*

Inlet Prerun/Postrun	The files that contain the optional GC pre/post run program parameters.
Parameter File (Process_Parms)	Optional Process parameter file. Available to external processes through the MLCURSMP.TXT file.
Process	Optional post-run program to be executed after acquiring this sample.
Process Options	Optional command line parameters for external Process when it is executed.
Vial	Specifies the Clarus 500 GC autosampler sample or bottle number for injection.

Sample Type

Sample type used during Quantify: Analyte, Standard, QC, or Blank.

An Analyte is a sample injection with unknown concentrations of target compounds.

A Standard is a sample injection with known, standard concentrations of target compounds.

A QC sample is used as a quality control measure to compare the calibration curve of the acquired data against a known concentration. The **QC** field in the Sample List has no effect on any calculations performed. When sample quantification is performed, the deviation of the analyte concentration is calculated against the QC concentration and this is shown as a percentage in the Quantify window under the heading %Dev. To select this heading, select **Conc. Deviation** from the Sample **Format** menu.

The value determined for a Blank sample is subtracted from future analyte runs. From the Quantify **Process** menu, select **Calculate**, and then select **Blank Subtract Compounds**. The quantification procedure checks through the Sample List and subtracts the concentration of each compound in a Blank from the corresponding concentration in an analyte. If several blanks are specified in a Sample List, then the preceding Blank is used for each analyte. If no Blanks are specified or there is no preceding Blank for the analyte of interest, then no Blank Subtraction is carried out. Blank Subtraction can only be done from the Quantify window. It cannot be done from the Sample List.

In addition the following Sample Types are added for **Environmental Reporting**:

- An **Analyte Duplicate (Analyte Dup)** is used when an Analyte is reprepared and reanalyzed. Typically the Sample ID remains the same.

- The **Tune Evaluation Sample (Tune Eval)** is an injection of BFB (4-Bromofluorobenzene) or DFTPP (Decafluorotriphenyl phosphine) used to verify that the mass calibration, mass resolution, and relative intensity of the mass spectrometer meets EPA-defined standard conditions. It might only contain the tune evaluation compound, or it might be part of the Continuing Calibration sample. It is typically analyzed every 12 hours.

- The **Initial Calibration (Init Calib)** is a multi-level calibration used to establish the quantitative calibration curves. In most environmental methods it is created when the mass spectrometer is new or cleaned. Thereafter on a 12-hour basis the Continuing Calibration is analyzed to verify that the Initial Calibration is still valid.

- The **Continuing Calibration (Cont Calib)** verifies that the Initial Calibration is still valid. It is typically a mid-level calibration sample. It is typically analyzed every 12 hours.

- A **Method Blank (Meth Blank)** sample is a blank used to verify the complete analytical procedure, including sample preparation. It is typically analyzed every 12 hours for VOA and every extraction batch of 20 samples for SV.

- The **Laboratory Control Sample (Lab Control)** is often similar to the Matrix Spike Sample, but spiked into a blank matrix (clean sand for soils or deionized water for waters) instead of a field sample matrix. It is typically analyzed every 12 hours.

- A **Matrix Spike (Spike)** sample is used to verify the quantitative extraction (recovery) of selected compounds (surrogates) from the sample matrix.

- The **Matrix Spike Duplicate (Spike Dup**) is a duplicate of the Matrix Spike sample, used to evaluate reproducibility.

- A **Dilution (Dilution)** sample is used when a sample's concentration exceeds the calibration range of the method. The sample is diluted. The surrogates are diluted in a SV sample, but not in a VOA.

- A **Re-Extraction (Re-Extract)** is a SV sample where the extraction procedure is suspect, and the sample is re-extracted.

Sample ID — An optional user-defined tracking number assigned to the sample.

NOTE: This field is filled in prior to acquisition if needed in the final reports. It cannot be changed after acquisition occurs.

Conc A-T — The concentration of a designated calibration level of compounds within a sample. Used during Quantify.

Job — Optional Job designation assigned to the sample. Recorded in the data file header.

Task — Optional Task designation assigned to the sample. Recorded in the data file header.

User — Optional TurboMass User identifier. Recorded in the data file header.

Submitter — Optional sample Submitter identifier. Recorded in the data file header.

Conditions — User comment on analysis and/or sample preparation conditions.

File Text — Optional Sample text description. Recorded in data file header.

Conditions
User comment on analysis and/or sample preparation conditions. Recorded in data file header.

User Divisor
Divisor used during concentration calculation stage of Quantify. Defaults to 1 if not specified.

User Factor 1…3
Multipliers used during concentration calculation stage of Quantify. Defaults to 1 if not specified.

Spare 1-5
General purpose fields to store extra information about the sample.

Quantify Method
The selectable method from the drop–down list. The list is populated with .mdb files from the <Project>\METHDB directory.

Calibration Curve
The selectable calibration curve file from the drop–down list. The list is populated with .cdb files from the <Project>\CURVDB directory.

Qualitative Method
The selectable method from the drop–down list. The list is populated with .qlm files from the <Project>\METHDB directory.

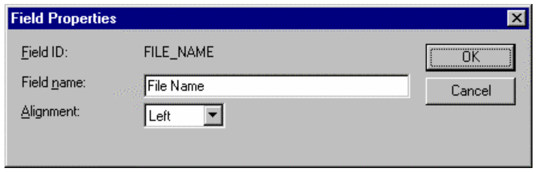
Report Method
The selectable method from the drop–down list. The list is populated with .rme files from the <Project>\METHDB directory.

3. To change the order in which the fields are displayed, select the name of the field, and click  or  until a field is in the required position.

4. To view field properties, select a column heading and click 

   OR

   Select **Properties from the Field** in the **Samples** menu to display the Field Properties dialog.



5. To change the name displayed at the top of the column, enter a new name in the **Field name** field.

6. To change the alignment of text in the column, select **Left**, **Right** or **Center** from the **Alignment** list.

   The text alignment in a cell, column, or row can also be changed by selecting the area, and clicking , , or , or selecting Left, Center or Right from the Align option in the Field option in the **Samples** menu.

7. To save a customized Sample List format, select **Save Format** from the **Samples** menu and enter a name in the dialog displayed.

8. To retrieve a previously saved format, select **Load Format** from the **Samples** menu, and select the required format from the list.

Selecting areas

You can select with the mouse, the keyboard, or a combination of both of these methods:

With the mouse:

To select:	**Left-click:**
A single cell	The required cell.
A block of cells	The first cell in the block, left-click and drag until the required cells are selected.
A row	The row number.
A column	The column heading.

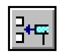
The entire Sample List	The box at the top left corner of the Sample List.

	ID	File Name
1	ID	Default
2	ID	Default

With the keyboard:

Position the cursor at the top left corner of the area to be selected, hold down the shift key, and use the arrow keys to select an area.

Inserting one or more rows

- To insert a single row, click .

  OR

  Select **Insert** from the **Samples** menu.

  OR

  Press INSERT.

To insert multiple rows, select the number of rows required and continue as for a single row.

Editing data in a cell

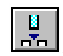
Do one of the following to edit data in a cell:

1. To select data for copying, replacing data, and other standard editing functions, select the cell using the mouse or press SHIFT+arrow key.

2. To edit a single cell, use the **Cut**, **Copy**, **Paste**, and standard Windows editing commands in the usual manner, or right-click to display the following pop-up menu.

Editing data in a column

The following commands may be used to edit data in a column:

Fill Down Select an area and click , or select **Down** from the **Fill** option from the **Samples** menu to fill the selected range with the first element in each column.

Fill Series

Select an area and click , or select **Series** from the **Fill** option from the **Samples** menu to fill the selected range with series data. That is, if the first cell in a column is vial1, the next will be vial2, vial3, and so on.

Insert

Click or select **Insert** from the **Samples** menu to insert samples into the Sample List. If a row has been selected, a new row is inserted above the current one. If more than one row is selected, the same number of rows is inserted above the first selected row. If a column has been selected, the same number of rows as were originally in the column are inserted before the first row. The data inserted into these new rows will continue the series from the row above.

For example, selecting the two highlighted rows in the figure on the left below and clicking **Insert** will result in the figure on the right.

	ID	Bottle
1	ID	Bottle
2	ID1	Bottle1
3	ID10	Bottle3
4	ID11	Bottle4

	ID	Bottle
1	ID	Bottle
2	ID1	Bottle1
3	ID2	Bottle2
4	ID3	Bottle3
5	ID10	Bottle3
6	ID11	Bottle4

If there is more than one number in a field, only the last number is incremented when **Fill Series** is selected. For example, if the ID is Sample1run1, when Fill Series is selected, the next field will be Sample1run2 etc.

The **Cut**, **Copy** and **Paste** commands can also be used to enter data. Select an area, **Cut** or **Copy** the data and **Paste** to a new area.

NOTE: *The Paste area must be same size as the Cut or Copy area.*

Replacing data in a cell

Use one of the following methods to replace data in a cell:

- Use the mouse or the arrow keys to select the cell, and enter or paste new data into the cell to replace the previous contents.

- Use the Cut, Copy, Paste and other editing commands, or right-click to display the following pop-up menu.

- Double-click on a cell, and select an entry from a drop-down list displayed.

- For Sample Type, select one of the displayed options.

- Select an entry from the list or enter in a new value.

- Enter in a new value.

Deleting rows and columns

➢ To delete a row, click  to delete the selected rows.
If the entire table is selected, the cells are cleared not deleted.

➢ To delete a column, select the column and click .

Starting the Analysis

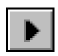
➢ Before starting an analysis save any changes made to the Sample List by selecting **Save** from the Sample List **File** menu.

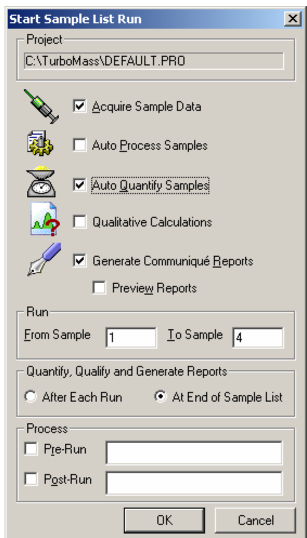
NOTE: *The GC status must be either "No Method" or "Run Done" to successfully set up. Otherwise GC communication lockups may occur.*

Acquiring data

1. Select **Start** from the TurboMass top level **Run** menu.

   OR

   Click  to open the Start Sample List Run dialog.



Project The name of the current project appears in this field. To acquire data to a different project, click OK or Cancel to exit

this dialog, open another project, and restart data acquisition.

Acquire Sample Data Selecting this option will acquire data for the specified samples in the list. See the Acquisition Help file (available in the **Help** menu) for more information on data acquisition.

Auto Process Samples Selecting this option will process the acquired data as specified in the Process column of the Sample List.

Auto Quantify Samples Selecting this option will automatically start sample quantification at the end of the Sample List.

Qualitative Calculations Selecting this option enables Qualitative Method Processing.

Generate Communiqué Reports Selecting this option enables Communiqué report generation.

Preview Reports Check this box to specify that the Communiqué reports generated during processing will be displayed in a preview window prior to printing (or saved to a file or database.

The options above allow you to acquire and immediately process and quantify data as desired. Or you may choose to process or quantify data at a later time.

Run From Sample To Sample Sets the range of samples in the sample list that will be acquired/and or analyzed. If you highlight a range of rows before starting the analysis, the first and last rows of the highlighted region will be displayed here.

Quantify, Qualify and Generate Reports

After Each Run This indicates specified processing will occur after each row in the sample List

At End of Sample List Indicates specified processing will occur only after the Sample List is complete.

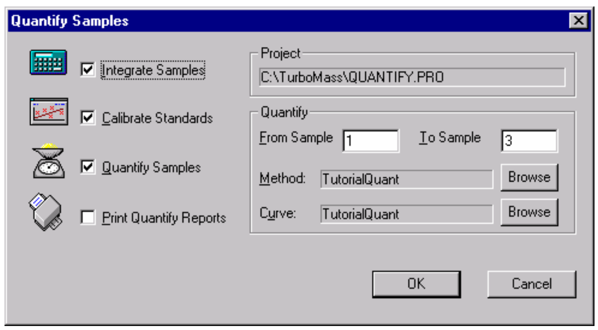
Process:

Pre-Run	Specify the name of the process that will be run before the acquisition of files in the Sample List
Post-Run	Specify the name of the process that will be run after the acquisition of files in the Sample List.

Quantify the Data

To quantify data after it has been acquired, select **Process Samples** in the Sample List **Quantify** menu.

1. Select the options required and click **OK** to start the analysis.

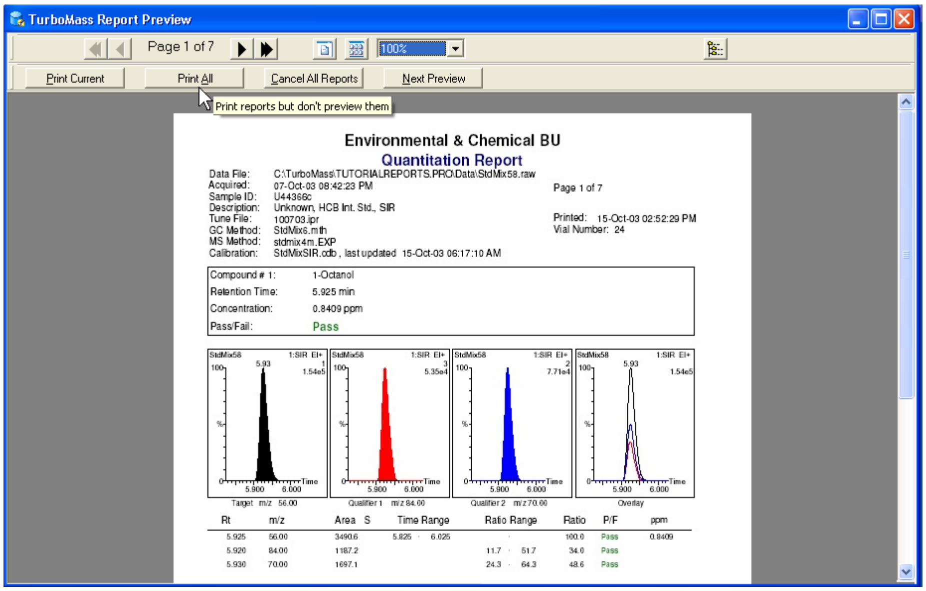


Integrate Samples	Integrates all the sample data files named in the peak list.
Calibrate Standards	Uses Integration results to form Quantify calibration curves from *all* the data files in the Sample List.
Quantify Samples	Uses Integration results and Quantify calibration curves to calculate compound concentrations from *all* the data files in the Sample List.
Print Quantify Reports	Produces hard copies of the results of integration and quantification.

Report Preview Window

This window displays when the Preview Reports option has been checked in the Start Sample List Run dialog and a Communiqué report has been generated as part of data reprocessing.

Only one report is available at a time in the preview window since each report is displayed when it is generated and further processing of the sample list is paused until the preview window is closed.

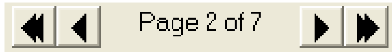
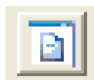
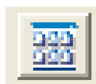
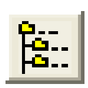


To review a report within this environment:

1. Use the page navigation and display tools to examine each page of the report.

Click the appropriate button to indicate the action settings regarding printing of the current report and previewing of future reports.

Main Report Preview Toolbar

Control	Description
	The text displays the number of the current page and the number of pages in the report. Either side of the text are buttons that display (from left to right): • The first page in the report • The previous page in the report • The next page in the report • The last page in the report.
	Displays a single page of the report in the preview area.
	Displays the drop–down palette from which a multi–page layout can be selected. Selection of a multi–page option will change the display in the preview area to that format (assuming the report contains sufficient pages).
	A drop–down list that enabled the user to select a zoom factor for the report display.
	Displays a standard Windows Save As dialog, enabling the user to save the current Communiqué data source as a file, which may later be loaded into the Communiqué Designer as preview data when editing templates.

Report Preview Action Toolbar

Control	Description
Print Current	A command button that prints the current report (where 'print' is defined within the Report Method) and closes the preview window. The next report from the sample list (if any) will be previewed.
Print All	A command button that prints the current report, enables printing for all future reports from the sample list (where 'print' is defined within the Report Method) and closes the preview window. Future reports will <u>not</u> be previewed.
Cancel All Reports	A command button that causes the preview window to close without printing the current report. Furthermore, future reports from the sample list will be neither previewed nor printed.
Next Preview	A command button that closes the preview window without printing the current report. However, the next report generated from the sample list (if any) will be previewed.

Quantify 10

Introduction

This section describes how to use TurboMass to perform quantitative assays. Many parts of the system are used to automate the acquisition, integration, quantification and reporting of data. The Quantify window is used to view the summary of Quantify results, calibration curves, and lists of integrated chromatography peaks.

TurboMass enables you to form Quantify calibration curves using Standard samples containing compounds of known concentrations. The calibration curves can then be used to calculate the concentrations of compounds in Analyte samples. For more information, see Appendix C *TurboMass Quantify Calculations.*

The results of Quantify can be viewed in the Quantify Summary window. Calibration curves can be viewed on the display and a number of Quantify Reports can be produced. Facilities are also provided for writing Quantify information to the Windows Clipboard for use by other Windows applications.

The TurboMass automated quantification provides a simple way of quantifying large numbers of samples within an analysis. Data can be acquired, processed, and reports printed without user intervention. The whole process is controlled from the Sample List Editor, which is a very important part of the Quantify system.

You provide a list of the samples and a Quantify method describing how to process each of the compounds within these samples.

Quantitative Processing for Environmental Analysis

Quantitative processing for environmental analysis is an extension to the TurboMass Quantify environment. The Communiqué data model is enhanced to support the additional data items required for environmental calculations.

It is also important to note that not all the calculations are performed by TurboMass Quantify, and some calculations are specific to certain sample types. Some calculations are only be performed when environmental reports are generated. These exceptions will be specifically noted.

Two principal categories of calculations can be identified for both volatile (VOA) and semi–volatile (SV) organic compound analyses:

- Matrix–specific concentration calculations
- QA/QC calculations (values associated with spiked samples

TurboMass Automated Quantification — an Overview

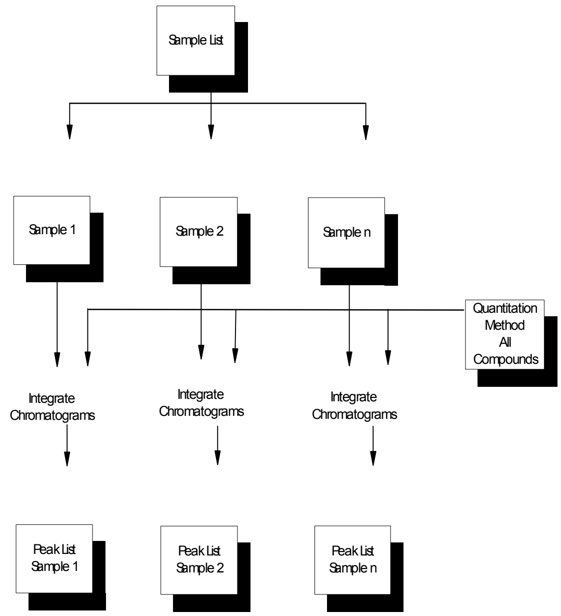
There are six basic stages in automated quantification:

1. Creation of a list of samples using the Sample List Editor.
2. Acquisition of each sample in the analysis.
3. Integration of data file chromatograms.
4. Formation of Quantify calibration curves.
5. Calculation of compound concentrations.
6. Printing reports of results.

How Does TurboMass Quantify and Report a List of Samples?

After data for all of the samples have been acquired, TurboMass must perform several tasks to get from a list of samples to a printed report of their concentrations. While you do have considerable flexibility in the control of these processes, quantification is still a straightforward operation, consisting of the following basic steps.

Integration of Chromatograms



Chromatogram integration is made up of two processes: smoothing and peak detection. You specify how these processes are to be applied in the Quantify method. The results of the peak detection are stored in a peak list that has the same name as that of the sample data file being processed.

The Sample List indicates which sample data files are to be integrated.

Each compound in the Quantify method specifies a chromatogram trace that is to be used to Quantify that compound. The chromatogram for each of the method compounds is integrated and the resulting peaks are saved to a single peak list.

Generation of Calibration Curves

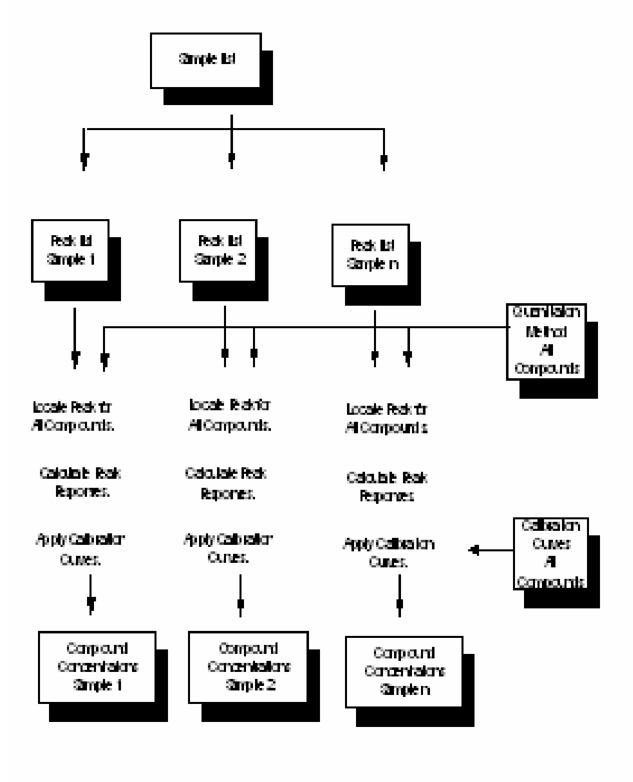
A calibration curve is formed for each of the compounds in the method. Samples that are to be used when forming a calibration are assigned the Standard type in the Sample List. The Sample List also specifies the concentration of each of the calibration standards.

The peak, which represents each compound, must be located within a sample's peak list. A response value for each of the located peaks can then be calculated. For located peaks, information such as compound name and peak response is saved in the peak list.

For each compound, one calibration point is obtained from each of the Standard peak lists. Calibration points are plotted as response against concentration. A polynomial is fitted to these points to form the compound's calibration curve. The calibration curves are saved to a file with the same name as the Quantify Method.

The Quantify Method specifies how to locate peaks, calculate responses, and fit curves.

Calculation of Compound Concentrations



TurboMass calculates the concentration of each of the Method compounds for the samples in the Sample List.

The peak, which represents each compound, must be located within a sample's peak list. A response value for each of the located peaks can then be calculated and saved along with the compound name and other peak information in the peak list.

A concentration is calculated for each of a compound's located peaks by applying the compound's calibration curve. Concentration information is saved in the peak list.

Displaying Quantify Results

Quantify displays the results of quantification in three windows.

Summary window Shows a list of results that can be ordered either by compound or by sample.

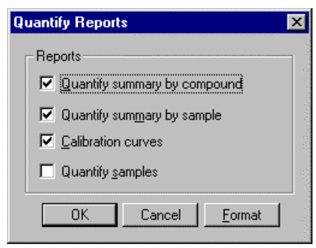
Graphs window Shows the calibration curve for each compound in the method with calculated statistics.

Peak List window Shows the information saved in the peak list for each sample.

The Summary window allows you to thoroughly examine the Quantify results.

To recall integrated chromatograms, double-click on a point in the summary, and modify baselines as necessary.

Reporting Results



Four printed reports of Quantify results are available:

Quantify Compound Summary Report Displays quantification results for each of the Quantify compounds ordered by compound.

Quantify Sample Summary Report Displays quantification results for each of the Quantify compounds ordered by sample.

Quantify Calibration Report Gives calibration curve graph for each Quantify compound.

Quantify Sample Report Graphically displays all located chromatogram peaks and tables quantification results. Report is grouped by sample.

NOTE: *The Chromatogram application is opened when producing the report.*

The Quantify Toolbar

The Toolbar is displayed at the top of the Quantify window. By choosing the toolbar buttons, you can perform some common operations.

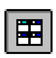
 Prints the current Quantify window display in portrait format.

 Prints the current Quantify window display in landscape format.

 Shows the previous peak in the Summary window.

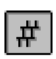
 Shows current peak in the Summary window.

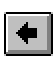
 Shows the next peak in the Summary window.

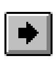
 Arranges the windows in a tiled view.

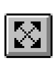
 Arranges the windows in a cascaded view.

 Arranges the windows in a stacked view.

 Selects the current entry.

 Decrements the current entry in the Summary window.

 Increments the current entry in the Summary window.

 Restores the default display range.

A Step-by-Step Guide to Quantification

Creating a Sample List

The first thing that you must do when using Quantify is to create a list of samples that you want to use to perform the analysis. These samples can be acquired manually, but more often they will be acquired automatically using an autosampler. The Sample List Editor has various columns such as Filename, vial or bottle Number and Sample Type that can be filled in for each sample. Each sample is displayed as one row in the Sample List. The Sample List Editor is part of the TurboMass top level menu.

You need to tell TurboMass everything that it needs to know about the samples in the list in order for it to perform a complete analysis. You must describe to the system what each of the vials in the autosampler contains; that is, whether it contains a standard, an analyte, a blank or a QC sample, how to acquire it, it and its concentration(s), if it is a standard. In addition, you must specify the name of the file in which to store the data. You may also want to add some management information such as Sample ID, the submitter's name, or a sample description.

For information on how to create a Sample List, see page 205.

Projects

TurboMass gives you the option to organize your work into projects. Projects are a very useful way of organizing all of the data files, methods and results for a particular assay into one directory structure on disk.

When you open a TurboMass project, TurboMass creates a new directory to hold all the different files associated with this project. The advantage of using projects is that it becomes very simple to archive everything associated with your assay because you do not have to hunt around the disk to find the files you need and the chances of you forgetting to save an important file are greatly reduced. You can save the following types of files in a TurboMass Project:

- Raw data files.

- Peak lists.
- Sample lists.
- Quantify methods.
- Quantify calibration curves.
- Tuning files.
- Scanning methods.
- Instrument calibration files.
- Inlet methods.

Projects are created and selected from the TurboMass top level **File** menu. See *Getting Started* on page 23 for instructions on how to create or open a Project.

Creating a Quantify Method

A Quantify Method must be created before Integration or Quantification can be performed.

The Quantify method describes how a data file is processed to produce calibration curves and quantitative information. Details must be entered into the method for each of the compounds being used in the analysis.

The Quantify Method specifies information for performing the following tasks:

- Integration of a chromatogram trace to obtain peak information.
- Location of the chromatogram peak relating to a specific compound from the list of detected peaks.
- Calculation of a response factor for the located peak.
- Formation of a Quantify calibration curve.
- Environmental calculations

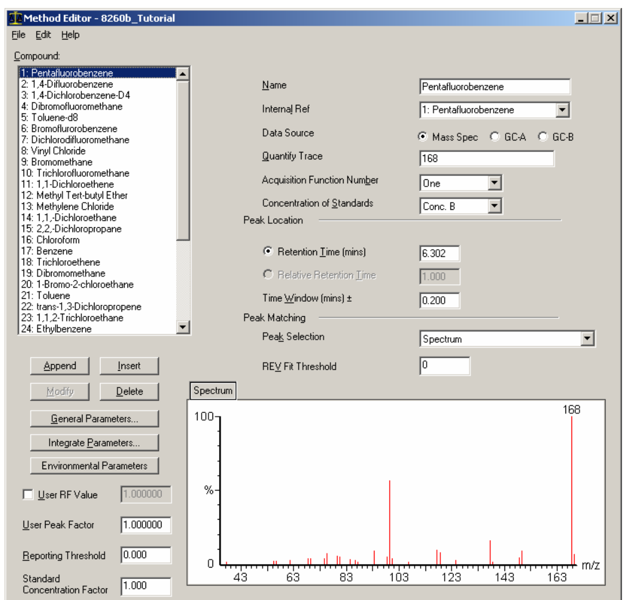
Quantify Method Editor

The Quantify Method Editor creates new methods and modifies existing ones. A method selected from within the Method Editor will become the current system method file and is used when performing Quantify operations.

Changes made to the method are not made permanent until they have been saved to disk. Consequently, the method must be saved before it can be used to perform quantification. This can be achieved by selecting **Save** from the File to update the current method file, or **Save As** to save to a new method file.

When opened, the Quantify Method Editor contains the current TurboMass method. If the current method is not available, the editor will contain default values, and the name of the current method in the editor title bar will be set to [Untitled]. The current method becomes the current system method file that is used when performing quantification.

➢ To open the Method Editor dialog select **Edit Method** from the **Quantify** menu.



Setting method parameters:

1. Enter the name of the compound in the **Name** field.

   The compound name can be up to 30 characters in length. The names of the compounds in the method appear in the **Compound** list.

2. Select the internal reference compound in the **Internal Ref** field. Set this parameter to **[None]** if the compound is not using an internal reference standard

   Only compounds that appear in the compound list can be selected.

3. Select the **Data Source** of the peak for the selected compound:

   - MS – Mass spectral data will be used
   - GC-A – The GC detector from channel A will be used (i.e., a .raw data file from this detector).
   - GC-B – The GC detector from channel B will be used (i.e., a .raw data file from this detector)

   If a GC detector is selected, most of the MS specific options will be deactivated (for For example, Quantity Trace, Acquisition Function Number, Relative Retention Time, REV Fit Threshold, and the Spectrum display).

4. Set **Quantify Trace** to the trace descriptor of the chromatogram being used to quantify the compound, as follows:

   - A single decimal number for mass chromatograms.
   - A range of masses (for example, 280 – 286 will sum the intensity of m/z 280 to m/z 286).
   - **TIC** for total ion current chromatograms.
   - **BPI** for base peak intensity chromatograms.

   The **Quantify Trace** parameter specifies a chromatogram to be integrated when TurboMass is performing automatic peak detection, and is used during the locate phase when TurboMass is matching peak list entries against method compounds.

Quantification on a selected mass chromatogram is usually preferred for sensitivity and selectivity. deally, the ion should be:

- Characteristic of the compound
- Have a high relative intensity
- A low background level
- As high in mass as possible - consistent with the previous requirements.

NOTE: *TurboMass enters this value automatically if you use the mouse to enter the Peak Location parameters. Be sure to verify that it is the best choice for avoiding co-eluting compounds. See* Peak Location parameters *in step 7.*

5. For multifunction data, select which function number is to be used to quantify the current compound from the **Acquisition Function Number** drop-down list.

6. Set the **Concentration of Standards** parameter to the Sample List column that contains the compound's concentration level within each Standard or QC sample.

   If the compound is an Internal Standard and it is at the same concentration in all samples, the **Fixed** option can be selected.

   The software allows up to 20 concentration levels within a single sample. For example, if one group of compounds is initially at 50 ppb, a second group is at 100 ppb, and a third is at 400 ppb, these three concentration levels can be defined as Conc. A, Conc. B, and Conc. C. As the standard is serial-diluted, change the values assigned to Conc. A, B, and C in the Sample List to reflect the new concentrations.

7. Set the **Peak Location** parameters to determine how a peak within a peak list is identified as matching a method compound. A peak can be classified as a match according to its Retention Time or Relative Retention Time, whether it falls within the specified Time Window, and whether it satisfies the Peak Selection criterion.

Retention Time	If selected, a peak within a peak list is identified as a match if it elutes at the Retention Time specified and within the Time Window specified.

Relative Retention Time	If selected, a peak within a peak list is identified as a match if it elutes at the time at which the compound is expected to elute relative to the compound specified in the Internal Ref text field.

8. Set the **Retention Time** or **Relative Retention Time** and **Time Window** parameters in one of the following ways:

   <u>Using the mouse:</u>

   a) Arrange the TurboMass display so that you can see both the Quantify Method Editor and the Chromatogram window showing the chromatogram you want to use.

   b) Select the **Compound** for which you want to set parameters in the Method Editor.

   c) Right-click at one end of the chromatogram region of interest, and drag the mouse horizontally to the other end. As you drag the mouse, TurboMass indicates the range you have selected. When you release the mouse, the Quantify Method Editor window will be updated to show the new **Time Window** and the **Retention Time** or **Relative Retention Time** will be set to the middle point of the **Time Window**.

   d) The **Quantify Trace** parameter will be set to the same type as the chromatogram selected with the mouse (TIC, BPI, or mass chromatogram).

   e) The **Retention Time** or **Relative Retention Time** parameters can also be selected by right-clicking the chromatogram on the peak apex.

      The spectrum may be inserted by copying it from the Spectrum window with Edit/Copy Spectrum List and then selecting the Edit/Paste Spectrum menu bar item in the Quantify Method Editor.

      If there is a significant degree of chromatographic or spectral background, the best approach to "purify" the spectrum is as follows:

      1. Perform a background subtraction in the Chromatogram window using the Process/Combine Spectra operations described in *Strip and Combine Functions* on page 461.

2. Edit/Copy Spectrum List in the Spectrum window.

3. Edit/Paste Spectrum in the Quantify window.

To remove specific contamination peaks from the spectrum, paste the spectrum into a text editor or spreadsheet and edit it before pasting it into the Quantify window.

Using the keyboard:

a) If **Retention Time** is selected, set it to the time in decimal minutes at which the compound is expected to elute, and set the **Time Window** parameter as described in step 7.

b) If **Relative Retention Time** is selected, set it to the time at which the compound is expected to elute relative to the compound specified in the **Internal Ref** field. The value specified here is a multiplication factor that is applied to the time at which the internal reference compound elutes. This can be used to handle situations where some drift may occur in the time at which compounds elute, but their relative retention times remain constant.

9. If you selected **Retention Time**, set **Time Window** to specify by how much the compound elution time may vary.

   The Time Window is applied either side of the predicted retention time to give a valid window. The Time Window also defines the chromatogram range that will be integrated.

10. Set **Peak Selection** to specify which peak should be located where more than one peak is detected within the time window. By default, the peak **Nearest** to the specified retention time will be selected. Other retention time-based options that can be selected are **Largest** peak and **First** peak or **Last** peak in the specified time window.

NOTE: *The setting for the Peak Selection control will determine the appearance of the lower part of the window.*

- Select **Spectrum** for the best match to the reference spectrum and specify the **Rev Fit Threshold** to do a reverse search test in peak selection. Only

peaks above the specified **Rev Fit Threshold** value are considered for the match. The REV Fit Threshold control will be enabled and the spectrum display will be visible.

NOTE: *Quantify does not perform background subtraction or AutoRefine during Spectral peak matching. . For example, when using spectrum data objects in a Communiqué report template, check the Spectrum Properties to make sure the Background treatment is set to None to match this behavior..*

- When you select **Multiple Ion Ratio - to Quantify Trace** the spectrum plot is hidden. The Qualifier Ion table, the Tolerance and the Coelution window controls will be visible. The REV Fit Threshold is enabled.

- When you select **Multiple Ion Ratio - to Base Peak** the spectrum plot control is hidden. The Qualifier Ion table, the Tolerance, Coelution window, Quantify Trace Target Ratio and Tolerance controls will be visible. The REV Fit Threshold is enabled.

- **any other selection** - The spectrum plot will be visible (and the multiple ion controls hidden) but REV Fit Threshold will be disabled.

11. Optionally specify the **User RF Value**. The User RF Value is used in cases where there are no calibration standards to plot a calibration curve. It represents the gradient of a curve and is used as a multiplication factor that will be applied to peak responses for the current compound to determine concentrations.

12. Optionally set the **User Peak Factor**. This value is a multiplication factor that will be applied to all calculated concentrations for the current compound. If the User Peak Value is left at zero or set to 1, the concentration values will not be changed.

13. Optionally set the **Reporting Threshold** value (in concentration units) to filter quantitative results in reports. This value is passed to Communiqué via the data source.

IMPORTANT: *The **Reporting Threshold value** will be used as the **Reporting Limit** for the purpose of setting flags on Form 1 and determining what Compounds to show for Compound on the general environmental Quantitative Report*

(PKIEnvQuant template) if no Custom Compound List (which includes Reporting Limits) is defined.

14. Optionally set the **Standard Concentration Factor** (Std Conc Factor). Set this parameter on a per compound basis and it is used by Quantify to adjust the concentration values in 'standard' samples in the sample list (including 'Init Calib' and 'Cont Calib') prior to calibration of the compound.

    Because TurboMass only provides for 20 unique concentration values (A thru T) in the sample list, an alternative mechanism is required for analyses (such as environmental work) where multi–level calibration of a large number of compounds can lead to the need for hundreds of distinct standard concentration values. The Standard Concentration Factor is the factor by which the designated concentration in the sample list (A thru T) must be multiplied in order to result in the actual concentration in the standard sample. Since only one Standard Concentration Factor'will be defined for each compound it is requirement that the standards will be prepared by serial dilution.

    Example of usage:

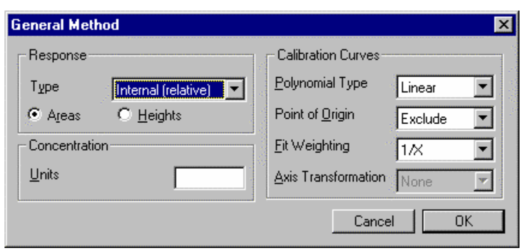
    Compound A specifies 'Concentration of Standards' = Conc A and has a 'Standard Concentration Factor' of 1.1155. The Calibration type is Linear Fit.

    The processed sample list includes four 'Standard' rows for which the contents of column A are 10, 20, 50 and 100.

    The actual concentration values used in generating the calibration curve (for graphic displays and for calculating the linear equation) will be:
    11.155, 22.31, 55.775 and 111.55.

Setting General Parameters

1. From the Quantify Method Editor dialog, click **General Parameters** to display the General Method dialog.



To use the General Parameters for all compounds in the method, select **Propagate General Parameters** from the Quantify Method Editor **Edit** menu. A check mark will appear next to this option, and the general parameters will be copied to all compounds in the method.

Response — **Response** parameters in the General Method dialog determine how the response value of a located peak is to be calculated. The response values are used to form calibration curves for compounds from standard samples and to calculate the concentration of compounds within analyte samples.

2. Set the Response Type to Internal (relative) or External (absolute).

   Select **Internal (relative)** if a compound's response is to be calculated using an Internal Standard, in which case, the **Internal Ref** parameters in the Quantify Method Editor must have the Internal Standard compound selected.

   Select **External (absolute)** if compound does not have an Internal Standard, the response is then taken as the absolute peak height/area.

3. Select **Response Areas** or **Heights** to specify whether the responses for the compound of interest will be based upon peak heights or areas.

   C**alibration** parameters in the General Method dialog determine how a compound's calibration curve is to be formed.

4. Select the type of calibration curve, **Average RF**, **Linear**, **Quadratic**, **Cubic** or **Quartic**, from the **Polynomial Type** drop-down list.

   Average RF — Produces a calibration, which is a straight line through the origin and through the mean response factor of the calibration points. A response factor is the response of a calibration point divided by its concentration. This option should be selected for compounds with a fixed concentration.

   Linear — Performs a linear regression on the compounds calibration points.

   Quadratic — Performs a second order regression on the compounds calibration points.

Cubic Performs a third order regression on the compounds calibration points.

Quartic Performs a fourth order regression on the compounds calibration points.

NOTE: *There must be one more calibration level than the order of the curve. For example, a linear curve needs two points, a quadratic curve needs three points, and so on. An* **Included** *or* **Forced** *origin counts as one calibration level.*

5. Select Point of Origin to Exclude, Include or Force.

   At the point of origin it is assumed that zero concentration has a response of zero. If **Polynomial Type** is set to **RF**, this parameter is not used.

   Force The calibration curve will always pass through the origin.

   Include The point of origin will be included in the calibration curve regression, the curve will not usually pass through the origin.

   Exclude The origin will be ignored when forming the calibration curve.

6. Set the calibration Fit Weighting to None, 1/X, 1/X^2, 1/Y or 1/Y^2.

   This parameter is used to give higher priority to calibration points with a low concentration or response when using regression to fit a calibration curve. This generally results in the calibration curve being fitted closer to points at low concentrations, thereby reducing the relative error at these points. Normally, this parameter is set to **None**.

7. Set the **Axis Transformation** parameter to the required option. The available options are **None**, **LN** (Natural Log), **Log** (Base 10 Log) and **Square Root**.

   The transformation is applied to the concentration and response values before the calibration curve is fitted. These transformations are useful with very wide dynamic range data to prevent all the low-concentration data points from being visually complressed together on the calibration curve.

   Axis transformations cannot be used with RF type curves, curves that use point weighting or curves that include or force the origin.

8. If required, set the **Concentration Units** parameter.

   The value set here will be used on the concentration axis of calibration curves and in the concentration column header in the Summary Report.

Mapping of Retention Time to Relative Retention Time

When **Retention Time** is the selected Peak Location mode and the compound has an Internal Reference defined, then the software will calculate the appropriate value for the 'Relative Retention Time' field and display it in that (disabled) field to 3 decimal places. The calculated value will be:

$$\text{RRT} = \frac{\text{RT (Current Compound)}}{\text{RT (Internal Reference)}}$$

When you enter a new value for RT the displayed RRT value will be updated when focus leaves the RT field.

Similarly, if **Relative Retention Time** is the selected Peak Location mode and the compound has an Internal Reference defined, then the software will calculate the appropriate value for the Retention Time field and display it in that (disabled) field. The calculated value will be:

$$\text{RT} = \text{RRT (current compound)} \times \text{RT (Internal reference)}$$

When you enter a new value for RRT the displayed RT value will be updated when focus leaves the RRT field.

If you change the compound defined as the Internal Reference for the current compound then the value in the selected/enabled Peak Location field will be used to calculate a new value to be displayed in the disabled field.

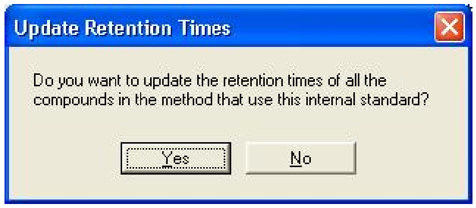
If a compound does not have an Internal Reference defined (or has one which is then changed to "[None]") then the RRT radio button will be disabled and the RRT field will remain disabled and blank.

Both RT and RRT values will be saved in the quantify method file. However, when the file is opened again in the editor only the 'active' data value will be read from the file, the other value will be calculated as described above.

Updating of Analyte RTs from Internal Reference

To simplify the process of updating retention times of analytes in complex quantify methods this option updates RTs of analytes when the RT of their internal reference peak is modified.

If the current compound is used as an Internal Reference by other compounds then when its RT is modified and you click the Modify button a dialog will be displayed asking you if the RTs of the associated analytes should be updated as well.



If you click the 'Yes' button then all compounds that use that Internal Reference (standard) will have their RTs modified according to the equation:

$$RTa' = \frac{RTi'}{RTi} \times RTa$$

Where:

RTa' is the new retention time of the analyte compound

RTi' is the new retention time of the internal reference (standard)

RTi is the old retention time of the internal reference (standard)

RTa is the old retention time of the analyte compound

When the updating is complete a dialog will be displayed indicating the number of compounds that were updated. This will act as a confirmation to the user that the action took place.

This same sequence of events will occur if you do not click the Modify button but respond 'Yes' to the 'Entry has been modified. Keep changes?" dialog displayed

after you have edited the Internal Reference RT and then select another compound or command.

Setting Multiple Ion Ratios

To set multiple ion ratios:

1. Select one of the ‘Multiple Ion Ratio’ options in the Peak Selection drop–down list.

    - Multiple Ion Ratio - to Quantify Trace

    - Multiple Ion Ratio - to Base Peak

2. Enter an appropriate REV Fit Threshold or leave the current value.

3. Enter m/z, Target Ratio and ±Tolerance for each of up to four qualifier ions in the grid,

    OR

    Paste in a spectrum previously copied from another environment. This action will automatically add m/z and target ratio values based on the data for the four highest-intensity ions (excluding the Quant ion). Default values for Tolerance will also be entered automatically. You may then edit any of these values if desired.

NOTE: *If the ‘Multiple Ion Ratio – to Base Peak’ is selected then Target Ratio and ±Tolerance values must be entered (below the grid) for the Quantify Trace.*

4. Accept the default Tolerance type or select the desired alternative from the drop–down list.

5. Accept the default Coelution Window value or enter the desired value.

Qualifier Ions

Type into the grid to define or modify the qualifier ions but the grid can also be filled in automatically using AutoBuild or by pasting a spectrum from the clipboard.

When the AutoBuild process is used (Chromatogram/Library Search Peaks etc.) the Paste Chromatogram command will have the following effect when the current setting of Peak Selection is 'Multiple Ion Ratio – to Quantify Trace' or 'Multiple Ion Ratio – to Base Peak'.

- The largest peak from the spectrum will be entered as the Quantify Trace, as occurs currently in TurboMass.

- The next four largest peaks will be entered as the qualifier ions. The Target Ratio values will be set according to the ratio of each ion to the quantify ion from the spectrum. The Tolerances will be set to the default value.

When the current setting of Peak Selection is 'Multiple Ion Ratio – to Base Peak' the Quantify Trace 'Target Ratio' will be set to its relative intensity in the pasted spectrum and the ±Tolerance will be set to the default value.

Pasting a spectrum will have the following effect when the current setting of Peak Selection is 'Multiple Ion Ratio – to Quantify Trace' or 'Multiple Ion Ratio – to Base Peak':

- The largest four peaks, excluding the Quantify Trace, will be entered as the qualifier ions. The Target Ratio values will be set according to the ratio of each ion to the ion indicated by the Peak Selection setting (i.e. to the Quantify Trace or to the Base Peak). The Tolerances will be set to the default value.

  m/z- Mass of the qualifier ion, displayed to two decimal places.

  Target Ratio- The expected intensity of the qualifier ion to the quant ion (as a %), displayed to one decimal place.

  ±Tolerance (%) - The variance permitted in the actual intensity ratio from the set Target Ratio, displayed to one decimal place. Use of this value is different depending on the tolerance type set in the Tolerance drop–down list.

  Quantify Trace: Controls for defining the Target Ratio and ±Tolerance for the Quantify Trace (where applicable).

  Tolerance - Control to set type of tolerance test applied to qualifier ions.

  Coelution Window (sec) ± - Control to set allowed time window for qualifier ions to maximize.

Setting Quantify Method Peak Integration Parameters

The Peak Integration parameters are used when automated chromatogram peak detection is being performed. You can set integration parameters for each compound or for all compounds within the method.

The facility to set different integration parameters for different compounds can be useful where peak characteristics such as peak width or shape vary between different compounds. For more detailed information on integration, see *Processing Chromatograms* on page 393.

Small peaks may optionally be removed by setting one of the four available threshold parameters: **Relative height**, **Absolute height**, **Relative area**, and **Absolute area**.

Setting quantify method peak integration parameters

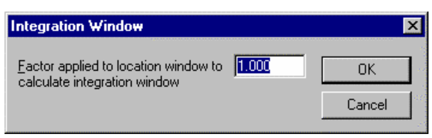
1. To use the same integration parameters for all compounds in the method select **Propagate Integration Parameters** from the Quantify Method Editor **Edit** menu.

   A check mark will appear next to this option and the integration parameters will be copied to all compounds in the method.

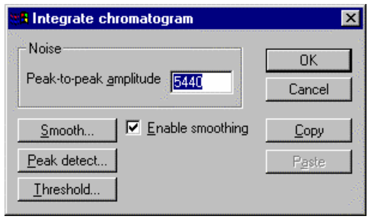
   By default, integration will take place over the chromatogram range defined by the **Time Window** parameter in the Quantify Method.

2. If you want to integrate over a larger window, select **Integrate Window** from the Quantify Method Editor **Edit** menu to open the Integration Window dialog, and specify a multiplication factor.

   This factor will be applied to the location window to calculate the integration window and is the same for all compounds in the method.

3. To define the integration parameters, click **Integrate Parameters** on the Quantify Method Editor dialog to open the Integrate chromatogram dialog.



4. Enter the **Noise Peak-to-peak amplitude** value used by the integration software to pre-filter the chromatogram by measuring a suitable value directly from a chromatogram.

5. Right-click and drag the mouse across a section of noise in the chromatogram. Then manually adjust this value to fine-tune the sensitivity of the integration algorithm.

   OR

   Enter a value into the **Peak-to-peak amplitude** field.

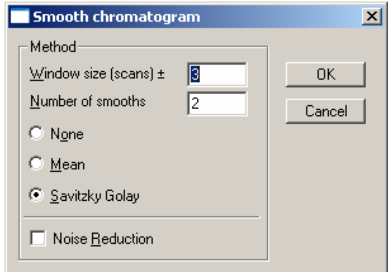
6. Click **Copy** and **Paste** as necessary to read and write integration parameters to and from the Windows Clipboard.

   This approach can be used to transfer integration parameters between Chromatogram and the Quantify Method, which can be useful when experimenting to find the correct integration parameters using Chromatogram.

Smoothing the chromatogram before integrating

1. Select the **Enable smoothing** checkbox.

2. To examine and edit the smoothing parameters, click **Smooth** on the Integrate chromatogram dialog to open the Smooth chromatogram dialog.



3. Set the **Window size** parameter to the half-width of the smoothing window in scans by right-clicking and dragging the mouse across a chromatogram peak or by entering a value in the field.

4. Set the number of times the smooth is repeated, by editing the **Number of smooths** parameter.

   Increasing this parameter gives a heavier smooth.

5. Select a Smoothing method.

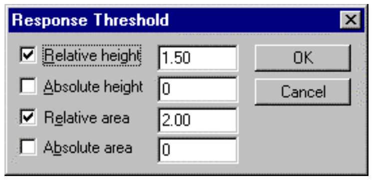
   Two types of smoothing are available for chromatograms; Moving **Mean** and **Savitzky Golay**. Both methods slide a window along the chromatogram, averaging the data points in the window to produce a point in the smoothed spectrum.

   Moving **Mean** takes the arithmetical mean of the intensities of the data points in the window.

   Savitzky Golay takes an average of the intensities weighted by a quadratic curve. This tends to enhance peak and valley shapes, as well as preserving the height of the peaks better than the Moving Mean. However, Savitzky Golay does tend to produce small artifacts on either side of the real peaks.

Setting peak thresholds

1. Click **Threshold** on the Integrate chromatogram dialog to open the Response Threshold dialog, and examine or modify these parameters.



2. Set the required parameters, and click **OK**.

Relative height Select if you want to remove peaks whose height is less than the specified percentage of the highest peak.

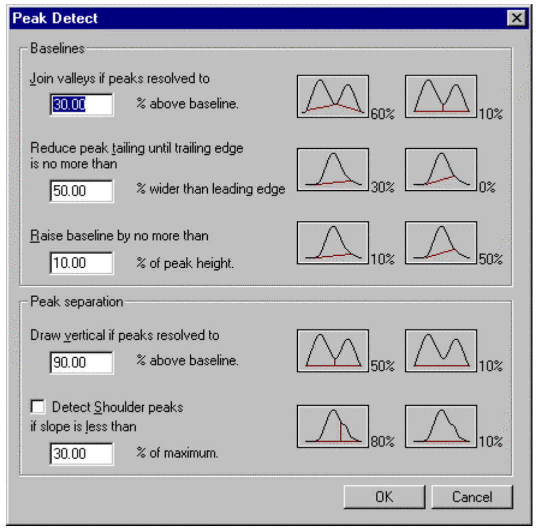
Absolute height Select if you want to remove peaks whose height is less than the specified value.

Relative area Select if you want to remove peaks whose area is less than the specified percentage of the largest peak area.

Absolute area Select if you want to remove peaks whose area is less than the specified value.

Setting peak detection parameters

1. You can examine and modify the parameters that control the positioning of baselines and separation of partially resolved peaks by verticals (droplines) by clicking **Peak detect** on the Integrate chromatogram dialog.



Join valleys Affects how baselines for partially resolved peaks are drawn. The larger the value of this parameter, the more peak baselines will be drawn up to the valleys between unresolved peaks. The default value for this parameter is 30 %, and normal operating range is 5 % - 75 %.

Reduce peak tailing and **Raise baseline** Allow control over the positioning of baseline end points. The default value for the reduce peak tailing parameter is 50 %, and normal operating range is between 25 % and 300 %. The **Raise baseline** parameter prevents the baseline end point from moving too high up the peak. To prevent the baseline endpoints from moving up the peaks, reduce the value of this parameter. The default value is 10 %, and normal operating range is 5 % - 20 %. This parameter is only relevant when the **Reduce peak tailing** parameter has a small value (less than 50 %).

Draw vertical Determines how well resolved peaks must be before they are separated by a dropline (or baselines are drawn up into the valleys, depending on the value of the Join valleys parameter). If you want poorly resolved peaks to be separated, increase the value of this parameter. The default value is 90 %, and normal operating range is 50 % - 100 %.

Detect Shoulder peaks You can optionally attempt to detect completely unresolved peaks, or shoulders, by selecting the Detect Shoulder Peaks checkbox. The algorithm will detect a shoulder if the slope of the shoulder top is less than the specified percentage of the steepest slope on the peak. Therefore, to make shoulder detection more sensitive, increase the value of this parameter. The default value is 30 %, and normal operating range is 20 % - 90 %.

Setting Environmental Reporting Parameters

The environmental parameters should not have to be changed frequently once established for the laboratory, however when changes are required it involves reviewing a large number of compounds. Using the Environmental Parameters dialogs makes interaction more convenient than the main dialog of the Quantify Method Editor by placing all the compound-specific environmental parameters in one place for quick viewing and editing.

The Environmental Parameters dialog displays the parameters based on the type of the currently selected compound; Target Compound, Surrogate Compound, Spike Compound, or Internal Standard Compound.

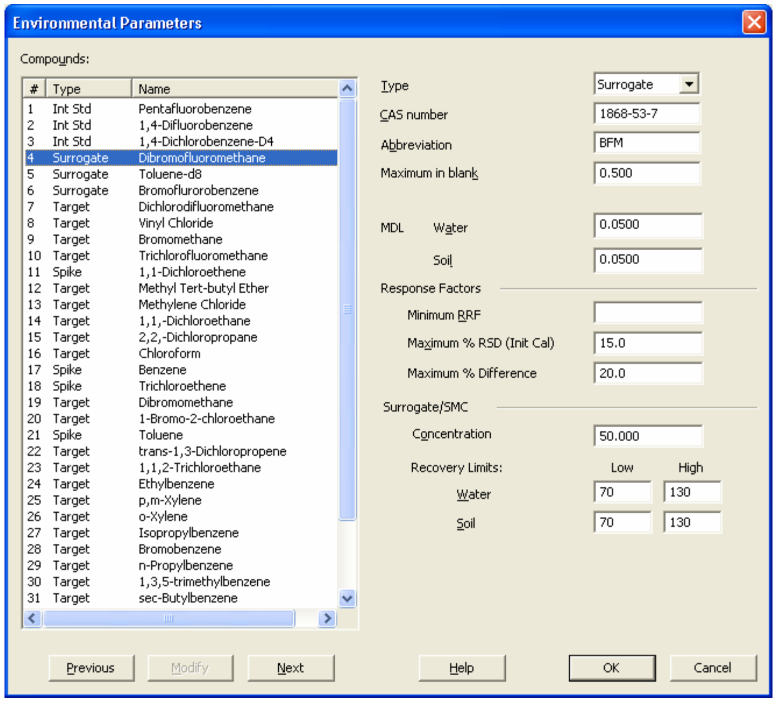
IMPORTANT: *Modifying any part of the Quantify Method may cause calculations to be invalid and we strongly advise against doing this without completely reprocessing (integrate, calibrate, quantify) the data.*

To set the environmental parameters for compounds:

1. In the Method Editor, select the first compound to be modified and click the **Environmental Parameters** button

   OR

   Choose **Environmental Parameters…** command in the Edit menu.



2. If the compound **Type** setting is not correct, select the appropriate value from the drop-down list on the right side of the dialog. In the above example the Type is Surrogate.

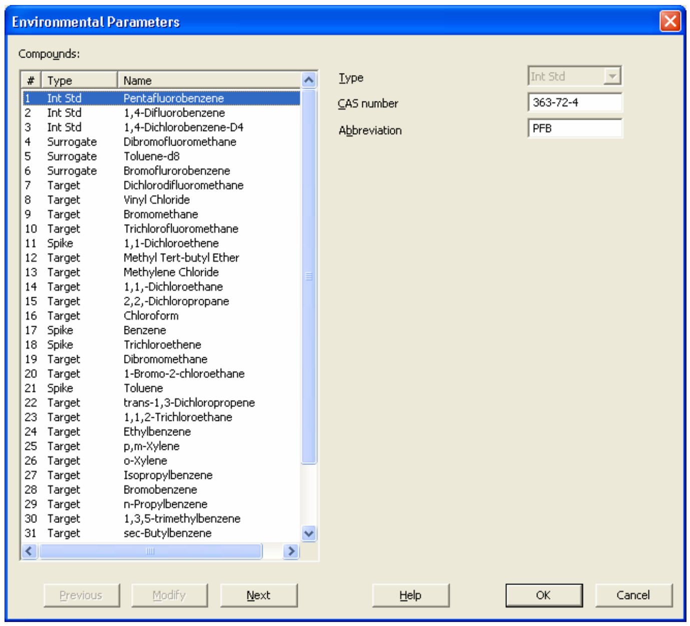
3. Modify numeric parameter fields as required.

4. Click **Modify** to accept the changes for the current component but leave it selected, or, click **Previous** or **Next** to accept the changes and move to a new component.

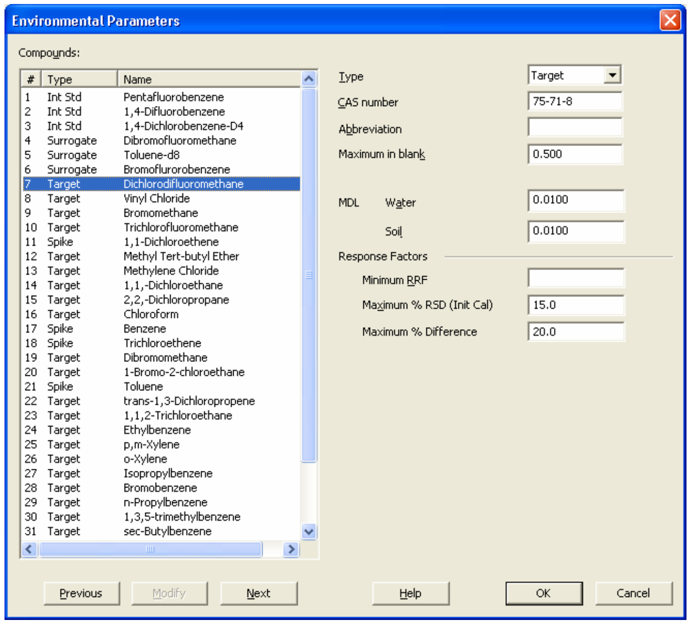
5. After making all required modifications, click **OK** to save the revised method (or **Cancel** to abandon all changes and leave the method unchanged).

Environmental Parameter Settings

The Environmental Parameters dialog displays when you click the **Environmental Parameters** button in the main Quantify Method Editor window (or choose the Environmental Parameters… command in the Edit menu). The specific form of the Environmental Parameters dialog depends on the type of the currently selected compound. If the Type is Internal Standard a dialog appears with the Type, CAS number and Abbreviation parameters.



If the Type is Target the following dialog appears:



Compounds: A list view of all compounds defined in the Quantify Method. The currently selected compound row will remain highlighted. The list displays:

- The compound number (this will be the same number displayed in the main Quantify Method Editor window). Clicking on # Sorts the compounds in the order in which they appear in the Quantify Method main window (or reverse order if clicked again).

- The compound type – Target, Spike, Surrogate or Internal Standard. (see also Type control). Clicking on Type sorts the compounds by type in alphabetical or reverse alphabetical order (or reverse alphabetical order if clicked again).

- The compound name, as it appears in the main Quantify Method Editor window). Clicking on Name sorts the compounds by name in alphabetical (or reverse alphabetical order if clicked again).

Type - A drop–down list that indicates the nature of the compound: Target, SMC/Surrogate, Spike, or Internal Standard.

NOTE: *A compound cannot be designated as an internal standard within this dialog. The use of a compound as an Internal Reference within the main Quantify Method Editor window defines it as an internal standard and will cause the Int Std selection to be displayed in this control as read–only.*

CAS number - An edit box specifying the Chemical Abstracts Service number for the compound.

Abbreviation - An edit box specifying the abbreviation to be used for the compound on Forms 2 and 8 (i.e., this is only used for Surrogates and Int. Stds.)

Maximum in blank - An edit box that indicates the maximum amount permitted (0.0000 to 9999.9999 or left empty) in the method blank before a 'B' flag will be assigned. If the concentration is larger than this value a 'B' flag will be assigned on Form 1 and Form 1 TIC.

NOTE: *"B" flags (indicating blank contamination) are not set when the compound concentration is less then the MDL. If you do not wish to see the "B" flag, you may set the Maximum in blank value equal to the Reporting Threshold.*

MDL: Water - An edit box to indicate the MDL (minimum detection limit) for the selected compound in water samples. Concentrations below this value will not be reported. This control is not available for internal standards.

MDL: Soil - An edit box to indicate the MDL (minimum detection limit) for the selected compound in soil samples. Concentrations below this value will not be reported. This control is not available for internal standards.

NOTE: *For the purposes of environmental reports, the term MDL is used to indicate the threshold value for the "U" qualifier flag. Values below this threshold value will flag the compound with a "U" in the Form 1 report and no concentration value will be printed.*

NOTE: *When using a Minimum Detection Limit (MDL) and Reporting Limit values, the TurboMass software handles the calculations for a straight dilution by using a dilution factor. However, if you modify the samples (e.g., volumes or weights) then you should refer to the EPA equations (specified in OLM04.2 or SOM11) to adjust the MDL and/or Reporting Limits for differences between the nominal (specified in the method) and the actual sample volumes and weights.*

Response Factors

For each target and surrogate compound you can define:

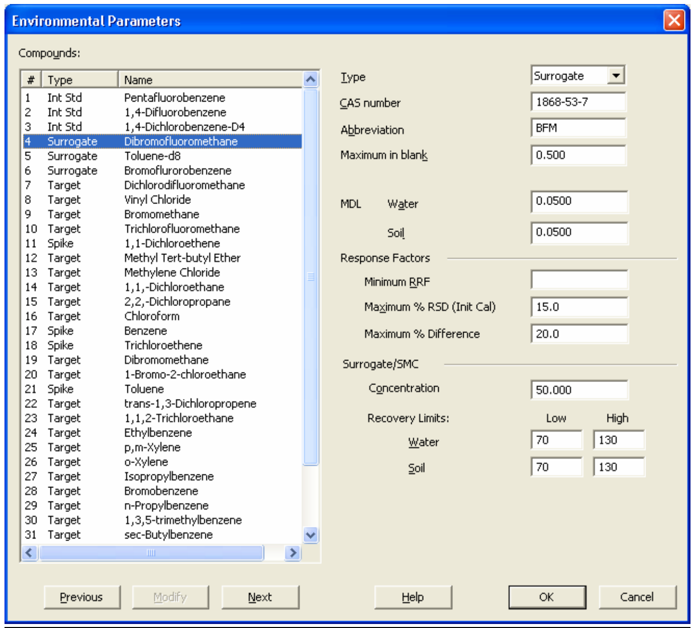
Minimum RRF - An edit box that defines the minimum acceptable RRF (Relative Response Factor to the internal standard) for this compound (0.0000 to 9999.9999 or left empty) in initial and continuing calibrations.

IMPORTANT: *If you change the **Minimum RRF** value, **Maximum % RSD** value and/or **Maximum % Difference** value, you **must reprocess (recalibrate)** the sample list for this new value to be used in the calibration acceptance testing.*

Maximum % RSD (Init Cal) - An edit box that defines the maximum acceptable % RSD (percentage relative standard deviation, 0.0 to 100.0 or left empty) between response factors calculated for each concentration level of the initial calibration.

Maximum % Difference [Maximum % Drift For compounds using curve fit] - An edit box that defines the maximum acceptable percentage difference between the RRF calculated for this compound from the continuing calibration and the average RRF from the initial calibration. For compounds using curve fit (e.g., linear least squares) this becomes the 'Maximum % Drift' – the acceptable difference between the concentration calculated for the compound in the continuing calibration standard using the calibration equation and the known concentration.

Surrogate/SMC



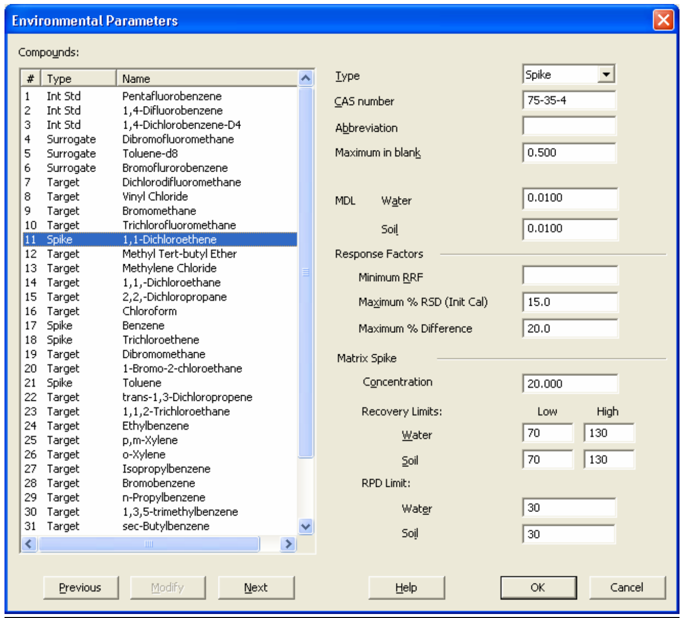
This dialog contains all of the above parameters plus the following:

Concentration - An edit box that defines the amount of the compound used to spike the sample.

Low Recovery limits: Water and Soil - An edit box that defines the minimum acceptable recovery percentage for the compound (spike or surrogate) in a Water sample and a Soil sample.

High Recovery limits: Water and Soil - An edit box that defines the maximum acceptable recovery percentage for the compound (spike or surrogate) in a Water sample and a Soil sample.

Matrix Spike



This dialog contains all of the above parameters plus the following:

RPD Limit for **Water -** An edit box that defines the maximum acceptable RPD (relative percent difference) value between the matrix spike and matrix spike duplicate recoveries, for water samples.

RPD Limit for **Soil -** An edit box that defines the maximum acceptable RPD (relative percent difference) value between the matrix spike and matrix spike duplicate recoveries, for soil samples

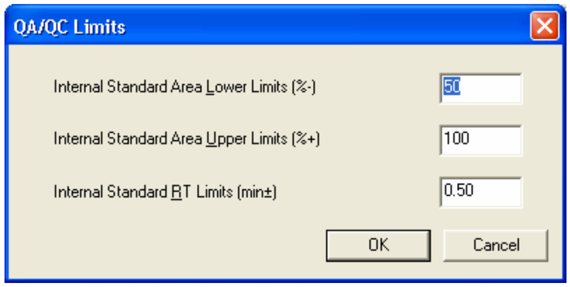
To Set QA/QC Limits

The QA/QC limits are a set of values that apply to all compounds (global parameters) in the method. For this reason the QA/QC Limits dialog is accessed from the Method Editor Edit menu rather than from a button in the compound list

section of the Method Editor since all items in this dialog are global to the method and not compound-specific.

To set QA/QC Limits:

1. From the Method Editor, select QA/QC Limits from the Edit menu.



2. Make the following entries then click OK.

   Internal Standard Area Lower Limit (% –) - The value (from 0 to 100) that defines the acceptable lower limit of the area measured for each internal standard peak in a sample, compared to that in the most recent continuing calibration, or mid–level of the initial calibration if no continuing calibration has yet been performed.
   Internal Standard Area Upper Limit (% +) - Enter a value (from 0 to 100) that defines the acceptable upper limit of the area measured for each internal standard peak in a sample, compared to that in the most recent continuing calibration, or mid–level of the initial calibration if no continuing calibration has yet been performed.
   Internal Standard RT Limits (min ±) - Enter a value (from 0.00 to 999.99) that defines the acceptable limits for the actual retention time of each internal standard peak in a sample, compared to that in the most recent continuing calibration, or mid–level of the initial calibration if no continuing calibration has yet been performed.

QA/QC Calculations

The following equations apply to both volatile and semi–volatile organics, and to all matrix types.

Recoveries

The recovery calculation shall be performed for each system monitoring compound/surrogate standard in all samples, blanks, matrix spikes and matrix spike duplicates.

$$\%\,\text{Recovery} = \frac{\text{Concentration (amount) found}}{\text{Concentration (amount) spiked}} \times 100$$

where:

Concentration (amount) found is calculated using the appropriate matrix specific equation
Concentration (amount) spiked is taken from the Quantify Method

Matrix Spike/Matrix Spike Duplicate Recovery

These calculations require that three data files be identified:

- An analyte sample (Analyte or Analyte Dup sample type in the sample list)
- A spiked sample that was prepared from the original analyte sample (Spike sample type in the sample list)

An optional third sample can also be identified.

- A second spiked sample prepared independently from the original analyte sample (Spike Dup sample type in the sample list)

NOTE: *Because these calculations require that the user has indicated unambiguously which three data files are involved, they will only be performed during the process of environmental report generation.*

The concentration of the matrix spike compounds is calculated using the same equations as used for the target compounds. The percentage recovery shall then be calculated as follows:

$$\text{Matrix Spike Recovery} = \frac{\text{SSR - SR}}{\text{SA}} \times 100$$

where:

SSR	Spiked sample result - calculated concentration from the Spike (Matrix Spike) or Spike Dup (Matrix Spike Duplicate) sample
SR	Sample result - calculated concentration from the unspiked Analyte sample
SA	Spike amount added - taken from the Quantify Method

The relative percent difference (RPD) of the recoveries of each compound in the matrix spike and matrix spike duplicate shall be calculated as follows:

$$RPD = \frac{abs(MSR - MSDR)}{½(MSR + MSDR)} \times 100$$

where:

MSR	Matrix spike recovery - calculated from the Spike and Analyte sample pair
MSDR	Matrix spike duplicate recovery - calculated from the Spike Dup and Analyte sample pair

Since the numerator is calculated from the absolute value of the difference between the recoveries, the RPD is always expressed as a positive value.

AutoBuild: Automatically Building a Quantification Method

After a chromatogram is labeled with the desired names, the names, retention times, spectra, and largest ion can be automatically used to build a quantification method. See the following procedure.

1. In Chromatogram, expand the time axis to the range of interest by dragging the left mouse button.

2. Select **Integrate** from the **Process** menu. Drag the right mouse button over a background range of the chromatogram to set the noise peak-to-peak amplitude.

3. Click **OK**. This will integrate the chromatogram.

4. Select **Lib Search Peaks** from the **Process** menu. Click **OK** when asked to print.

NOTE: *To save paper, you can pause the printer, and later delete the contents of the print queue. See* Avoiding Printout of Library Search Results *on page 389.*

5. When library searching is complete, return to Chromatogram and select **Copy Detected Peaks** from the **Edit** menu.

NOTE: *If* **Display Peak Name** *is selected, the peak name, if available, will be displayed above the peak. (To select* **Display Peak Name***, select* **Peak annotation** *from the Chromatogram* **Display** *menu.) For more information on using names to label the chromatogram, see* Annotation Type Parameters *on page 388*.

6. Open the Quantification method by selecting **Edit Method** from the Sample List **Quantify** menu.

   It may be a new or exisiting method.

7. Enter the **Time** window you wish to use.

8. Select **Paste Chromatogram** from the **Edit** menu.

   The library search name, the largest ion, the retention time, and the spectrum will be entered into the method.

9. You may now enter any compound-specific information, such as **Internal Ref.** Verify that the Quantify ions are those you wish to use.

10. Save the method.

AutoUpdate: Automatically Updating Retention Times in the Quantify Method

To automatically update the retention times in the Quantification method:

1. In the Sample List, select **View Results** from the **Quantify** menu.

2. In Quantify, select **View** from the **Display** menu.

3. Select **Show Summary Window** and **List by Sample** in the Summary section, and then click **OK**.

4. Select the data file of interest by pressing the left or right arrow icons.

5. Remove any undesired peaks by double-clicking on the peak name and pressing DELETE, and then click **OK**.

6. When you are ready to update the Quantification method with the retention times in the list, select **Update Retention Times** from the **Process** menu.

CAUTION	*The update is immediate and irreversible.*

Creating a new Quantify method

1. Select **New** from the **Quantify File** menu.

   The editor parameters are set to default values, and the **Compound** list is empty. The name of the current method in the editor title bar is set to [Untitled].

2. Add the desired compounds as described below.

3. Select Save As from the Quantify File menu. Enter the name of the new method into the Save As dialog.

Selecting an existing Quantify method

1. Select **Open** from the Quantify **File** menu.

2. Select the required method file from the file selection dialog, and click **Open**.

   The compounds within the method appear in the **Compound** list. The first compound in the method is selected.

Propagating general parameters to all compounds

➢ To use the same integration parameters for all compounds in the method, select **Propagate General Parameters** from the Quantify Method Editor **Edit** menu.

A check mark will appear next to this option and the general parameters will be copied to all compounds in the method.

Propagating integration parameters to all compounds

➢ To use the same integration parameters for all compounds in the method, select **Propagate Integration Parameters** from the Quantify Method Editor **Edit** menu.

A check mark will appear next to this option and the integration parameters will be copied to all compounds in the method.

Adding a new compound

1. Enter the required information for a new compound.
2. Click **Append** to add the new compound to the end of the compound list.

Inserting a new compound

1. Select the entry in the compound list before which the new compound is to be inserted.
2. Enter the required information for the new compound, and click **Insert**.

Modifying information for an existing compound

1. Select the entry in the compound list that is to be modified.
2. Enter the updated information, and click **Modify**.

Deleting a compound

1. Select the entry in the compound list that is to be deleted.
2. Click **Delete** or press DELETE to remove the selected compound from the list.

Deleting all compounds in the method

1. Select **Delete All Compounds** from the Method Editor **Edit** menu.

2. Click **OK** to delete all compounds in the method.

Printing a Quant Method Report

You can print out Method data in two compressed formats.

1. Select **Print Table** from the Quantify **File** menu.

2. Select the desired options in the Print Method Report dialog:

Sort By The table may be sorted by retention time, compound name, internal reference standard, or the quantify trace ion.

Report Type The Compact format displays the compound data in paragraph format, taking as many lines for the compound as required. The Extended format displays one compound per line.

Compound Select **Current** to display the current compound. Select **All** to display all compounds

OR

Select **Range** and enter the compound range in the text field.

3. Optionally, enter text for the headers and footers on the report.

4. Select **Page Numbers** to add page numbers to the report.

Editing the Compound Format in the Quantification Method Report

Selecting which fields will be displayed in the Quantification Method Report

➢ Select **Edit Compound Format** from the Quantify **Edit** menu to display the Report Format dialog.

The fields present in the Method Report are shown in the **Displayed Fields** list in the Report Format dialog. Other fields that can be added to the Method Report are displayed in the **Available Fields** list.

The Method Report will display up to the maximum number of columns that will fit on one page. To include more columns, print in landscape mode instead of portrait mode.

Appending new fields to the Method Report

1. Select the field you want to append in the **Available Fields** list box.
2. Click **Append**.
3. Repeat steps 1 and 2 as required.
4. Click **OK** to save the changes.

Inserting new fields in the Method Report

1. Select the field you want to insert in the **Available Fields** list.
2. Select the field before which you want to insert the new field in the **Displayed Fields** list, and click **Insert**.
3. Repeat steps 1 and 2 as required.
4. Click **OK** to save the changes.

Removing a field from the Method Report

1. Select the field you want to remove in the **Displayed Fields** list.
2. Click **Remove**.
   To remove all the fields in the Method Report, click **Remove All**.
3. Repeat steps 1 and 2 as required.
4. Click **OK** to save the changes.

Formatting the display of a field in the Method Report

1. Select the field whose display settings you want to change in either the **Available Fields** or **Displayed Fields** lists.

2. Change the **Header** field to display the heading you want to display above this column.

3. Change the **Justification** setting to **Left**, **Right** or **Center** as required.

4. Change the **Field Width** and **Decimal Places** as required.

5. Repeat steps 1 through 4 as required.

6. To change the settings for all fields back to default values, click **Default**.

7. Click **OK** to save the changes.

Starting the Analysis

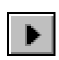
➢ Before starting an analysis save any changes made to the Sample List by selecting **Save** from the Sample List **File** menu.

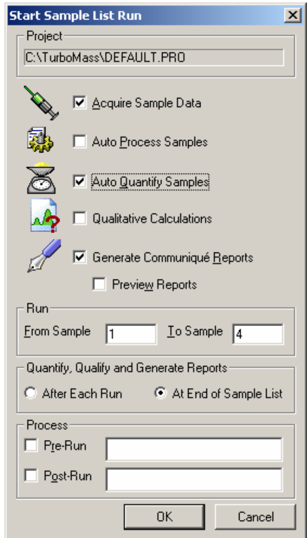
NOTE: *The GC status must be either "No Method" or "Run Done" to successfully set up. Otherwise GC communication lockups may occur.*

Acquiring data

2. Select **Start** from the TurboMass top level **Run** menu.

   OR

   Click  to open the Start Sample List Run dialog.



Project	The name of the current project appears in this field. To acquire data to a different project, click OK or Cancel to exit this dialog, open another project, and restart data acquisition.
Acquire Sample Data	Selecting this option will acquire data for the specified samples in the list. See the Acquisition Help file (available in the **Help** menu) for more information on data acquisition.
Auto Process Samples	Selecting this option will process the acquired data as specified in the Process column of the Sample List.
Auto Quantify Samples	Selecting this option will automatically start sample quantification at the end of the Sample List.
Qualitative Calculations	Selecting this option enables Qualitative Method Processing.
Generate Communiqué Reports	Selecting this option enables Communiqué report generation.

Preview Reports Check this box to specify that the Communiqué reports generated during processing will be displayed in a preview window prior to printing (or saved to a file or database.

The options above allow you to acquire and immediately process and quantify data as desired. Or you may choose to process or quantify data at a later time.

Run From Sample To Sample Sets the range of samples in the sample list that will be acquired/and or analyzed. If you highlight a range of rows before starting the analysis, the first and last rows of the highlighted region will be displayed here.

Quantify, Qualify and Generate Reports

After Each Run This indicates specified processing will occur after each row in the sample List

At End of Sample List Indicates specified processing will occur only after the Sample List is complete.

Process:

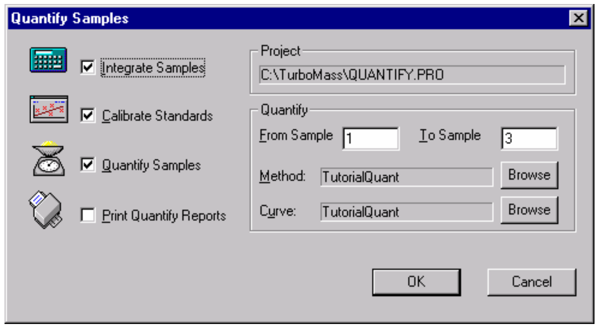
Pre-Run Specify the name of the process that will be run before the acquisition of files in the Sample List

Post-Run Specify the name of the process that will be run after the acquisition of files in the Sample List.

Quantify the Data

To quantify data after it has been acquired, select **Process Samples** in the Sample List **Quantify** menu.

2. Select the options required and click **OK** to start the analysis.



Integrate Samples Integrates all the sample data files named in the peak list.

Calibrate Standards Uses Integration results to form Quantify calibration curves from *all* the data files in the Sample List.

Quantify Samples Uses Integration results and Quantify calibration curves to calculate compound concentrations from *all* the data files in the Sample List.

Print Quantify Reports Produces hard copies of the results of integration and quantification.

Quantify From Sample To Sample Sets the range of samples in the sample list that will be quantified.

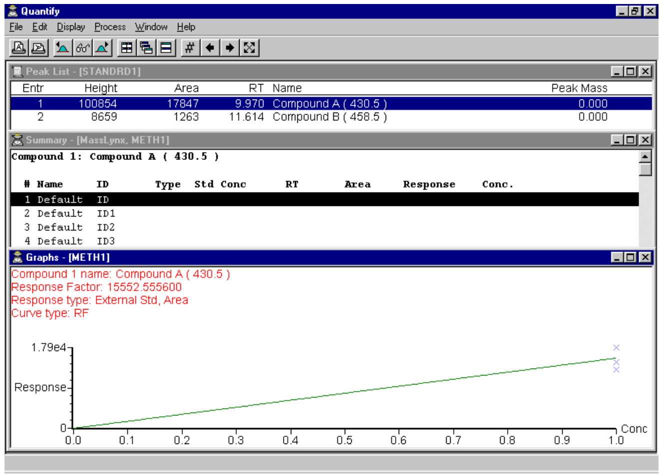
Using the Quantify Window to Examine Results

The Quantify window contains three windows: the Summary window, the Graphs window, and the Peak List window. You can turn each of these on and off as required.

NOTE: *If a peak is missed in Quantify because of retention time or ion ratios, it is necessary to manually integrate it before the Quantify/View Results/Process/Update Retention Times/Ion ratios can be used for it.*

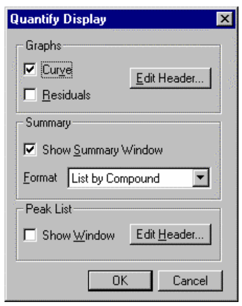
Displaying the Quantify window

➢ Select **View Results** from the top level **Quantify** menu.



Controlling the appearance of the Quantify display

1. Select **View** from the Quantify **Display** menu to display the Quantify Display dialog.



2. Specify the Quantify windows you want to display by selecting the appropriate checkboxes.

   You can choose to display any combination of the following: the Graphs window showing calibration curves, the Graphs window showing residuals, the Summary window, and the Peak List window.

3. Choose whether you want to display the Summary window listed by compound or by sample, by selecting the relevant setting from the Summary **Format** drop-down list.

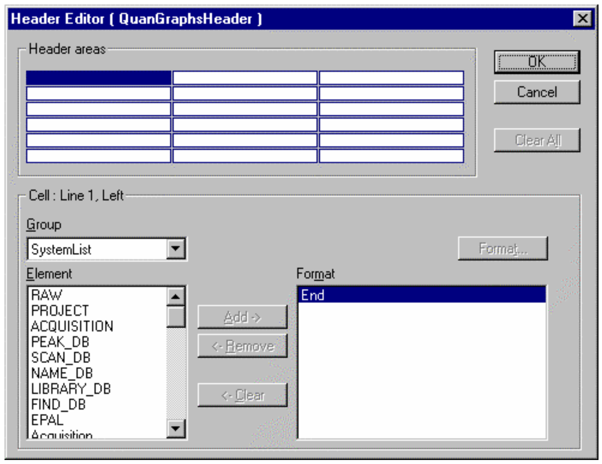
A user configurable header can be displayed at the top of the Graphs or the Peak List windows. In the default display the header is not displayed.

4. To open the Header Editor dialog, click **Edit Header** from the View dialog.

   OR

   Open the Header Editor from outside the View dialog by selecting an existing header.

   See *The Header Editor* on page 54 for more information about using the Header Editor.



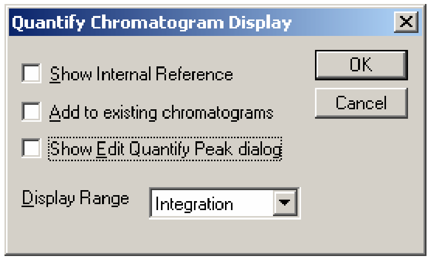
Controlling the appearance of the Quantify Chromatogram display

1. To display a particular peak list entry in the Chromatogram window select the desired entry in the Summary window or the Peak List window entry.

2. To display a particular calibration standard peak, select the desired calibration point in the Calibration Curve window. This allows manual adjustment of integration results.

3. To control the appearance of the Chromatogram window, select **Chromatogram** from the Quantify **Display** menu to open the Quantify Chromatogram Display dialog.

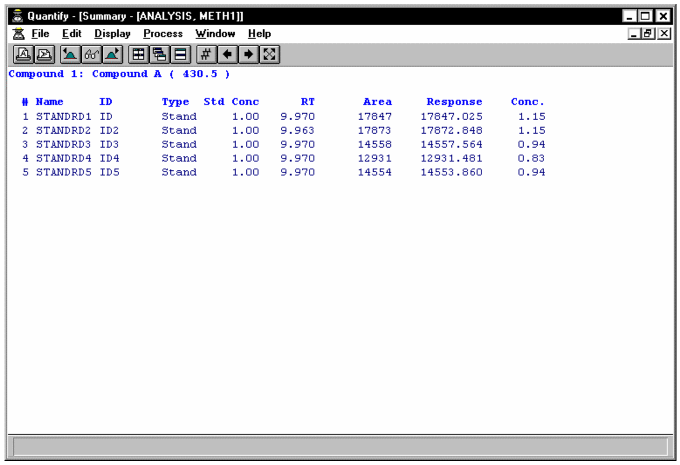
4. Edit your parameters.



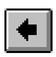
Show Internal Reference	If selected, the internal reference peak (if specified) will be shown with the current peak.
Add to existing chromatograms	If selected, each new chromatogram will be added to those already displayed.
Show Edit Quantify Peak Dialog	If selected, the dialog enables you to edit the Quantify Peak.
Display Range	Can be set to Integration to use the integration range, Keep Current to keep range currently displayed, or Acquisition to use the acquisition range.

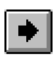
The Summary Window

The Quantify Summary window gives a summary of the results of quantification. The results in the Summary window can either be listed by compound or by sample. If no peak has been located for a compound entry, the peak information fields will be left blank.



Use the Quantify toolbar buttons to display information about a new compound/sample.

 Shows previous compound/sample in Summary window.

 Shows the next compound/sample in Summary window.

The Quantify Toolbar buttons can be used to display integrated peaks in Chromatogram.

 Shows the previous peak in the Summary window.

 Shows the current peak in the Summary window.

 Shows the next peak in the Summary window.

The Summary window format also determines the format of printed Summary Reports. Two Summary Reports can be printed: the Summary Report listed by sample, and the Summary Report listed by compound.

There are many different columns of quantification information that can be displayed in the Summary window. You can select which columns are currently displayed. Use the horizontal and vertical scroll bars, if available, to move around the Summary window.

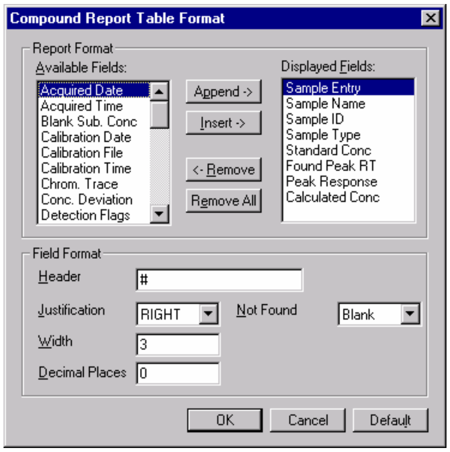
The format of the Summary window listed by sample and listed by compound can be changed independently.

The fields present in the Summary window are shown in the Displayed Fields list in the Compound Report Table Format dialog. Other fields that can be added to the Summary window are displayed in the Available Fields list.

Any changes made in the Compound Report Table Format dialog will be reflected in the Summary window display and in the Summary Reports. The Summary Reports will display up to the maximum number of columns that will fit on one page. To include more columns print in landscape mode instead of portrait mode.

Selecting which fields will be displayed in the Summary window and Summary Reports

Select the **Summary window column headers**, **Output Compound Format**, or **Output Sample Format** from the Quantify **Edit** menu to display the Compound Report Table Format dialog.



Appending new fields to the Summary window

1. Select the field you want to append from the **Available Fields** list.
2. Click **Append**.
3. Repeat steps 1 and 2 as required.
4. Click **OK** to save the changes and update the Summary window.

Inserting new fields in the Summary window

1. Select the field you want to insert from the **Available Fields** list.
2. Select the field before which you want to insert the new field in the **Report Format** list, and click **Insert**.
3. Repeat steps 1 through 2 as required.
4. Click **OK** to save the changes and update the Summary window.

Removing a field from the Summary window

1. Select the field you want to remove in the **Report Format** list.
2. Click **Remove**.
   To remove all the fields in the Summary window, click **Remove All**.
3. Repeat steps 1 and 2 as required.
4. Click **OK** to save the changes and update the Summary window.

Formatting the display of a field in the Summary window

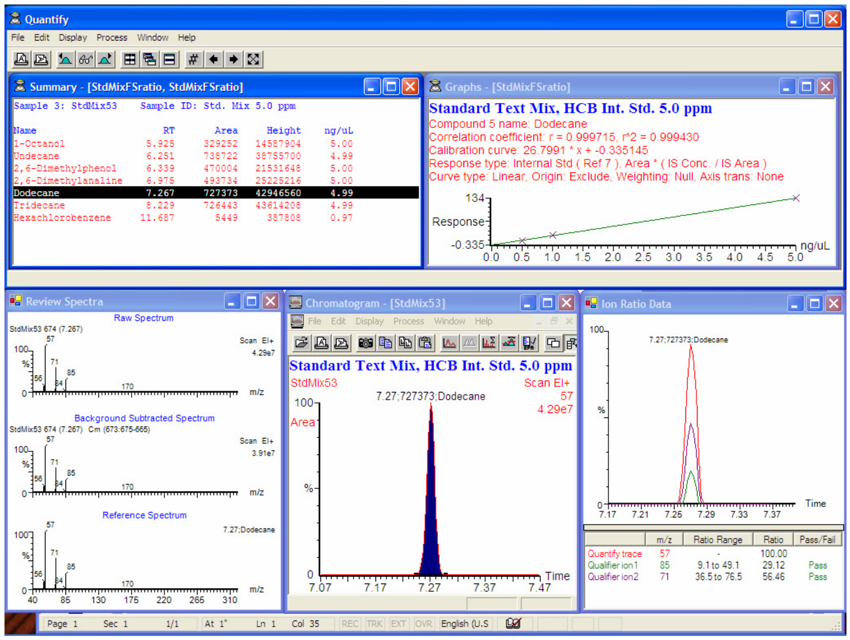
1. Select the field whose display settings you want to change in either the **Available Fields** or **Displayed Fields** list.
2. Change the **Header** field to display the heading you want to display above this column.
3. Change the **Justification** setting to **Left**, **Right** or **Center** as required.
4. Change the Field **Width** and **Decimal Places** as required.
5. Change the **Not Found** parameter as required.
   Not Found determines what will be printed in the Quantify report for this field if the peak is not found. The options available are **Blank**, **Zero**, **Dash**, **Not found or n/a**.
6. Repeat steps 1 through 5 as required.
7. To change the settings for all fields back to default values, click **Default**.
8. Click **OK** to save the changes and update the Summary window.

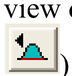
Reviewing Target Compound Data (Interactive Data Review)

To review target compound data:

1. Open the Quantify window by choosing the View Results… command from the Quantify menu.

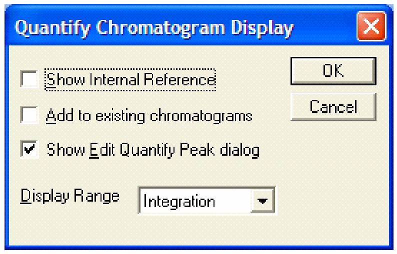
2. With the Summary window (by Sample) displayed, double–click on a peak to view the chromatogram, spectra and qualifier ion plots associated with that peak.



3. To view data for the next (or previous) peak click the toolbar button:  (or )

To modify peak data:

1. Double-click on the compound name in the Summary window you wish to manually integrate.
2. If the Edit Quantify Peak dialog is not displayed, select Chromatogram from the Display menu in Quantify and make sure the Show Edit Quantify Peak dialog is selected. Then try step 1 again.



3. Perform manual reintegration, if necessary. See Manual Peak Integration on page 311

4. Click OK to accept the changes made and have the results display updated.

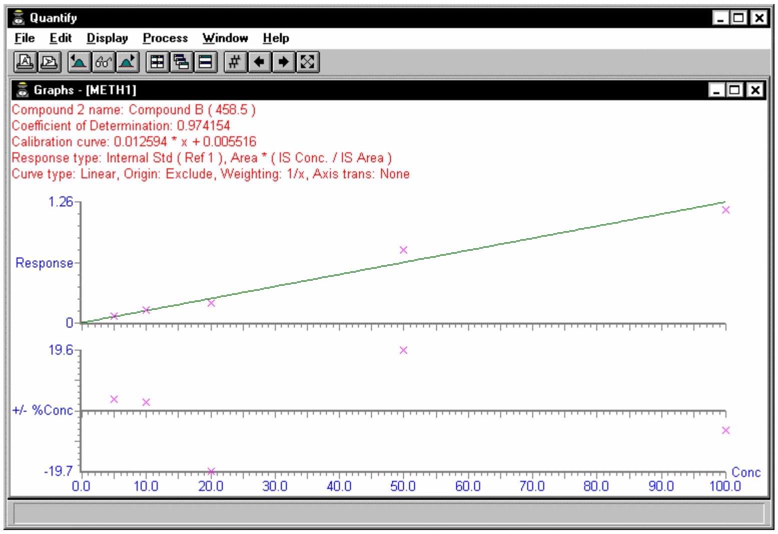
Saving the Summary window

In the Summary window, select **Save Summary by Compound** or **Save Summary by Sample** from the **File** menu.

The Graphs Window

The Quantify Graphs window contains a graphical display of the current calibration curve and/or its residuals plot. Statistical information on the calibration curve is displayed above the graphs. A user configurable header can be displayed at the top of the window.

The Graphs window is available if you selected **Curve** and/or **Residuals** in the Quantify Display dialog.



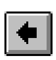
The current calibration curve file holds a calibration curve for each of the compounds being analyzed. The toolbar within the Graphs window allows you to easily select other calibration curves by clicking  or .

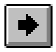
The calibration curve graph displays concentration against response value. The vertical axis is labeled as a percentage of the maximum response. The horizontal axis is labeled with the concentration units specified in the method. The displayed calibration curve shows the response value expected for particular concentrations. Crosses mark the calibration points used to form the curve.

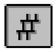
The residual plot displays concentration against delta concentration at the calibration points. This shows the difference between the concentration predicted by the calibration curve and the actual concentration at the calibration points.

Selecting another calibration curve

To select another calibration curve from within the current file, use the following tool buttons:

 To show the previous calibration curve.

 To show the next calibration curve.

 To open a dialog where you can enter the number of the desired calibration curve. Curve number 1 is for the first compound, curve number 2 the second, and so on.

Changing the display range of the calibration curve

Both the horizontal and vertical display ranges of the Graphs window can be expanded.

1. Left-click and drag the mouse horizontally, vertically, or diagonally from one end of the region of interest to the other.

   As you drag the mouse, TurboMass indicates the range you have selected. When you release the mouse, the selected range will be redisplayed to fill the current window.

   Repeat this operation as often as required.

2. To restore the display to the default range, click .

Viewing another calibration curve file

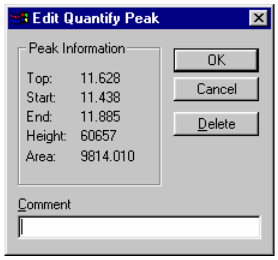
1. Select **Calibration** from the **File** menu to open the File Open dialog.

2. Select a file, and click **Open**.

Displaying more information about a particular calibration point

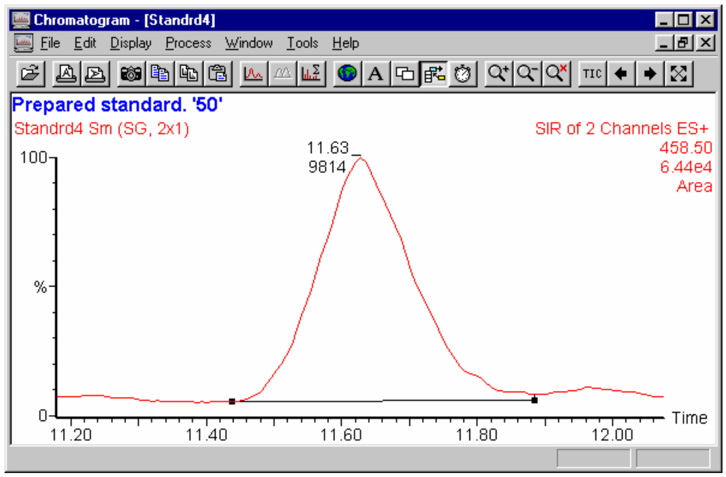
1. Select a calibration point to update the Summary and Peak List windows to display the calibration point as the current entry.

2. Double-click on a calibration point to display the peak list entry, display the corresponding chromatogram, and open the Edit Quantify Peak dialog.



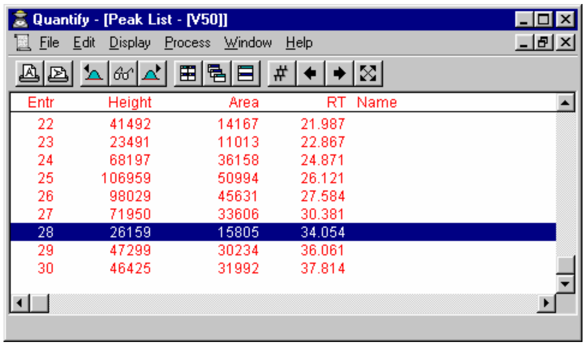
3. Manually adjust the baseline assignment as necessary.

4. Add any **Comment** that you want to store in the peak list for the selected peak. For more information, see Manual Peak Integration on page 311.



The Peak List Window

Select **Show Window** from the Quantify Display **View** menu to display the Peak List window.



The Quantify Peak List window lists all the peaks in the current peak list with the current peak selected. You can configure the columns displayed in the Peak List and the header displayed at the top of the Peak List window.

The Peak List window displays all the information for a peak list entry. To accommodate display space restrictions, you can select which columns are to be displayed and the order in which order they are to appear.

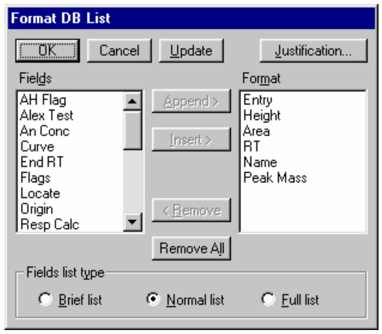
Configuring the displayed Peak List columns

To select Configure Peak List columns:

1. Select **Peak List Display Format** from the Quantify **Display** menu to open the Format DB List dialog, and then select the desired column(s).

   OR

   Use the mouse to select the desired column headings in the Peak List window.



Appending new fields to the Peak List window

1. Select the field you want to append from the **Fields** list.
2. Click **Append**.
3. Repeat steps 1 and 2 as required.
4. Click **OK** to update the Peak List window.

Inserting new fields in the Peak List window

1. Select the field you want to insert from the **Fields** list.
2. Select the field before which you want to insert the new field in the **Format** list.
3. Click **Insert**.
4. Repeat steps 1 to 3 as required.
5. Click **OK** to update the Peak List window.

Removing a field from the Peak List window

1. Select the field you want to remove from the **Format** list.
2. Click **Remove**.

To remove all the fields in the Peak List window, click **Remove All**.

3. Repeat steps 1 and 2 as required.

4. Click **OK** to update the Peak List window.

Formatting the display of a field in the Peak List window

1. Select the field whose display settings you want to change in either the **Fields** or **Format** list.

2. Click **Justification** to open the List Field Justification dialog.

3. Change the **Field Name** to show the heading you want to display above the column.

4. Select the **Justification** setting to **Left**, **Center** or **Right** as required.

5. Edit the Field **Width**, Significant Figures (**SF**) and Decimal Places (**DP**) as required.

6. Click **OK** to update the Peak List window.

Changing the Current Peak List file

➢ To view another Peak List, select **Peak List** from the **File** menu to display the File Open dialog, and select a peak list.

Displaying Peak List Chromatograms

➢ To display the chromatogram and peak associated with a Peak List window entry, double-click on the desired entry.

Manually Changing Quantify Results

Although TurboMass can perform a complete automated quantification analysis from setting up a Sample List and acquiring data to printing Quantify Reports, it is also possible to repeat individual Quantify processes and to manually edit results including:

- Manual editing of peak baselines.
- Editing calibration curves to exclude erroneous calibration points.
- Performing Quantify Locate compounds, Calculate calibration curves or Quantify compounds processes.

Manual Peak Integration

If the automated peak detection is not determining peak baselines satisfactorily, it is possible to define the baselines manually. This can be achieved by modifying the peak information held in the Peak Lists or by creating them from scratch.

1. To display an integrated peak in Chromatogram, select the desired entry in the Summary window or the Peak List window entry.

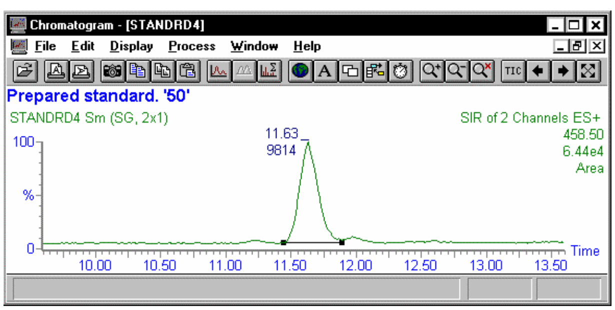
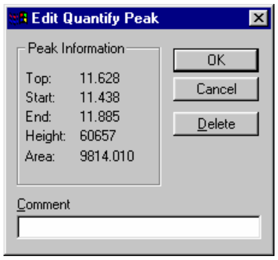


Figure 9 Chromatogram showing peak used for a calibration point

2. To display calibration standard peaks, double-click on the desired calibration point in the Calibration Curve window.

   TurboMass opens the Chromatogram window with the relevant peak displayed. Also, the Edit Quantify Peak dialog is opened. This displays detailed peak information and from which you can manually adjust the baseline.

3. To modify the peak baseline, select the handles that appear at either side of the baseline, and adjust the baseline as required.

   TurboMass will update the **Peak Information** displayed in the Edit Quantify Peak dialog.

4. When you are satisfied with the manual integration, click **OK** to save the new peak integration information.

5. Optionally, add a **Comment** to be stored in the peak list for the selected peak.

   The comment can be included in the printed report.

6. If no peak was detected, the chromatogram that should have contained the peak can be displayed by using the mouse to select the appropriate Summary window entry.

7. To add a baseline, right-click at one end of the chromatogram region of interest, and drag the mouse horizontally to the other end.

   As you drag the mouse TurboMass indicates the selected range. When you release the mouse, a baseline will be drawn.

8. To delete the current peak, click **Delete** and then **OK** in the Edit Quantify Peak dialog.

The peak list and associated windows will be updated. If the peak is a calibration standard, you will be asked if you want to recalculate the calibration curve. If a new curve is calculated, all compounds will be requantified.

The Summary window can be formatted to include the Detection Flags for each peak. The Detection Flags give information about the start and end points of the peak and can have the following values:

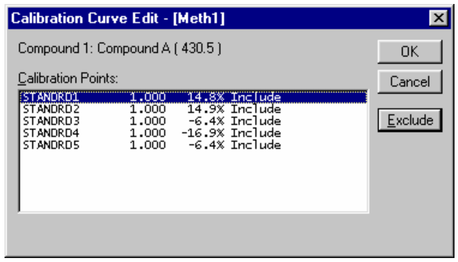
b	Peak baseline starts or ends on the chromatographic curves
v	Peak starts or ends as a valley dropline between two peaks
s	Peak baseline starts or ends as a shoulder dropline between two peaks
M	Peak start or end point has been manually assigned
t	Peak end was not detected within the retention time window
X	Calibration point has been excluded from the calibration curve

The default Chromatogram display range can be controlled by selecting **Chromatogram** from the Quantify **Display** menu. For more information about setting the default Chromatogram display range, see *Controlling the Appearance of the Display* on page 385.

Excluding erroneous calibration points

If, once the calibration curves have been formed, a calibration point is seen to be erroneous, it can be removed from the calibration as follows:

1. Select **Calibration Curve** from the Quantify **Edit** menu to open the Calibration Curve Edit dialog.



The Calibration Curve Editor will display a list of the calibration points used to form the calibration curve. Each point is displayed with Peak List name, standard concentration, residual error %, and a label to indicate whether the point has been included or excluded from the current calibration curve.

2. To exclude a point that is currently being used to form the calibration curve, select the calibration point in the list and click **Exclude**.

   The label for the point will change from **Include** to **Exclude**.

3. To include a point that is not currently being used to form the calibration curve, select the calibration point in the list and click **Include**.

   The label for the point will change from **Exclude** to **Include**.

4. When you have finished making changes, click **OK** to save the changes.

   You will be asked if you want to quantify compounds according to the new calibration curve.

5. Click **Yes** to quantify compounds or **No** to keep the existing calculated concentrations.

   The calibration curve will be replotted using only the included calibration points. Excluded points are denoted by a circle around the point. Excluded points are denoted in the Summary reports with an X in the Detection Flags column.

Excluding a complete sample from being used to form the calibration curve

If, once the calibration curves have been formed, all calibration points from a particular standard sample are seen to be erroneous, the sample can be removed from the calibration as follows:

1. Determine which sample produced the erroneous calibration points.

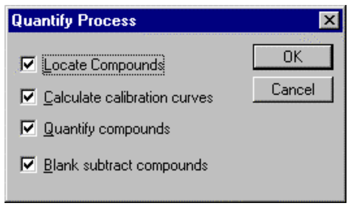
2. In the Sample List Editor, find the row that contains the erroneous sample and set the **Type** field to **Blank**. Alternatively, remove the row from the Sample List.

3. Click **Start**, and select the **Calibrate**, **Quantify** and **Print Report** options. There is no need to integrate again.

4. Click **OK** to start the analysis.

Performing any of the Quantify processes

1. Select **Calculate** from the Quantify **Process** menu to open the Quantify Process dialog.



2. Select the Quantify processes you want to perform:

Locate Compounds	Locates peaks for all compounds in the current method.
Calculate calibration curves	Plots calibration curves for all standards.
Quantify compounds	Calculates concentrations for analyte samples using the current calibration curves.
Blank subtract compounds	When a sample defined as a blank is encountered, the value is saved and subtracted from subsequent samples until the next blank is encountered, this new value is saved and subtracted from the next set of samples.

3. Click **OK** to exit.

Controlling Quantify Reports

Four printed reports of quantification results are available:

Quantify Compound Summary Report: Displays quantification results for each of the Quantify compounds ordered by compound.

Quantify Sample Summary Report: Displays quantification results for each of the Quantify compounds ordered by sample.

Quantify Calibration Report: Gives calibration curve graph for each Quantify compound.

Quantify Sample Report: Graphically displays all located chromatogram peaks and tables quantification results. Report is grouped by sample.

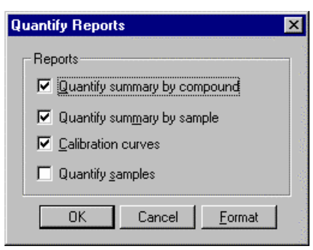
NOTE: *The Chromatogram application is opened when producing the report.*

Printing Quantify reports

1. Quantify Reports will be automatically printed at the end of a sample list analysis if **Print Quantify Reports** is selected when a sample list analysis is started.

   OR

   Select **Print Report** from the Quantify **File** menu to open the Quantify Reports dialog.



2. Choose the reports you want to print by selecting the appropriate checkboxes.

3. Click **OK** to save changes and open the Print dialog.

4. Set the print and print setup parameters as required.
   The Quantify Report margins can be changed by clicking **Margins**.

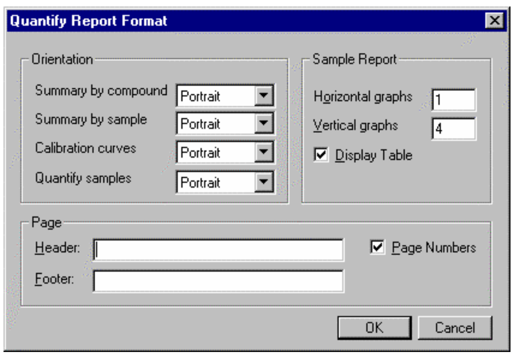
5. Click **OK** to print the Reports.

Changing the format of the Quantify reports

1. To open the Quantify Report Format dialog, either select **Report Format** from the Quantify **File** menu.

   OR

   Select **Print Report** from the Quantify **File** menu to open the Quantify Reports dialog, and then click **Format**.



2. Enter the required text in the **Header** and **Footer** fields to create a customized header and/or footer that will appear on each page of the Quantify Reports.

3. Select or deselect **Page Numbers** to turn page numbering on or off as required.

4. Set the **Sample Report** parameters to specify the number of **Horizontal graphs** and **Vertical graphs** you want to display on one page of the Sample Report.

5. If you want to print out a summary table of the sample results as well as the graphs, select **Display Table**.

6. Set the **Orientation** to **Portrait** or **Landscape** for each part of the Quantify Report.

7. Click **OK** to exit and save the changes.

Selecting which fields are displayed in the Quantify Summary Reports

➢ Select **Output Compound Format** or **Output Sample Format** from the Quantify **Edit** menu.

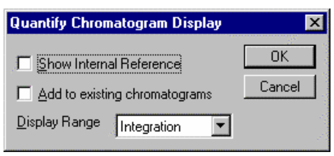
For more information about formatting Summary Reports, see Selecting which fields will be displayed in the Summary window and Summary Reports on page 238.

Selecting the Chromatogram display range for the Quantify Sample Report

The Quantify Sample Report uses the Chromatogram display parameters.

1. To set the Chromatogram display parameters, select **Chromatogram** from the Quantify **Display** menu.

   The Quantify Chromatogram Display dialog is displayed.



2. Select **Show Internal Reference** if you want the internal reference peak shown with the current peak.

3. Select **Add to existing chromatograms** to display each new chromatogram to those already on display.

4. Set the **Display Range** to **Integration** to use the integration range or to **Acquisition** to use the acquisition range.

If the Display Range is set to **Keep Current**, TurboMass will use the acquisition range.

Printing Quantify windows

1. Select **Print** from the Quantify **File** menu.

2. Select to print **All Windows** or **Current Window** and click **OK** to print the Quantify windows.

Printing Quantify windows using the Quantify toolbar

 Prints the current Quantify window display in portrait format.

 Prints the current Quantify window display in landscape format.

Writing Quantify Summary to the Clipboard

Quantify allows the equivalent of the Quantify Summary Report to be written to the Clipboard. From there, the information can be pasted into other applications, such as a spreadsheet. Quantify uses the currently selected Sample List, Method and Peak List files.

The Quantify Summary Report can either be ordered by compound or by sample.

To write the Quantify summary information to the clipboard, select **Copy Summary By Compound** or **Copy Summary By Sample** from the Quantify **Edit** menu.

Files Used During Quantify

Four types of files are used by the Quantify program: **Sample List**, **Method**, **Peak List** and **Calibration Curve**. The current file of each type can be selected from the Quantify **File** menu. It is recommended that you use the Projects option when doing quantification as this allows you to organize and access your data more easily. For more information, see Projects on page 47.

The Sample List (.SPL) File

Three items in the Sample List are required for quantification.

File Name: Specifies the sample data file name, which will be the same name as the corresponding Peak List file.

Type: Specifies the type of sample. This should be set to Standard if the sample is to be used to form a calibration curve, Analyte if the concentration of the compounds within the samples is to be calculated, QC if it is a quality control sample, or Blank if the sample does not contain any analyte compounds.

Concentration: Only required if the sample is a standard and is optional for QC samples. Specifies the known concentrations of the compounds within the standard. This does not apply to compounds whose concentration has been specified as being constant, (fixed), within all samples.

The Sample List files are normally stored in the \SAMPLEDB directory.

The Quantify Method (.MDB) File

The Quantify Method contains an entry for each of the compounds being analyzed determining how the data are to be processed. The same method is applied to all the samples in the analysis. For more information, see *Creating a Quantify Method* on page 257.

The Method files are normally stored in the \METHDB directory.

Peak Lists (.PDB) File

A Peak List contains peaks that were detected when integrating chromatograms. Further information gathered as a result of running Quantify, such as compound name and concentration, is also saved in the peak list.

Peak lists are produced as a result of running the TurboMass automated Quantify software or by the Chromatogram application. One peak list should be formed for

each of the samples in the analysis. The peak list will have the same name as the sample from which it was formed.

For more information on examining, modifying and creating peak lists, see *Chromatogram* on page 365.

The peak list files are normally stored in the \PEAKDB directory.

Calibration Curves (.CRV) File

Stores the Quantify Calibration Curves that are produced for each of the compounds within the method. The Calibration Curve file has the same name as the method used to create it.

The Calibration files are normally stored in the \CURVEDB directory.

Qualitative Method 11

Introduction to Qualitative Processing

You can determine the identity of your sample through the qualitative processing of sample data. To do this you create a Qualitative Method of the data (that you can specify) in each row of the Sample List. This defines the parameters required for generating reports that do not make use of quantitative results. The parameters fall into two main categories:

1. Definition of input data for generating a peak data set

2. Library search parameters

Qualitative processing can have one or two stages:

1. Integration of one of more defined chromatograms to generate a peak list.

2. Automatic library searching of the peak spectra and reporting of potential 'hits' The first step will always be carried out if a qualitative method is specified in the Sample List. The output of this process will be a collection of peak data which can be made available to Communiqué as a data source for qualitative reports and/or used as input to the automatic library search.

The first step will always be carried out if a qualitative method is specified in the Sample List. The output of this process is a collection of peak data which can be made available to Communiqué as a data source for qualitative reports and/or used as input to the automatic library search.

Qualitative Integration and Peak Selection

Only the number of peaks specified by the 'Report largest n peaks' parameter in the Qualitative Method will be included in the data source. The steps in the processing are:

1. Integrate each chromatogram.

   The specified trace (TIC or mass) will be extracted from the specified acquisition

function. Peak detection and integration are carried out in the manner it is done in the TM Chromatograms environment. Threshold values will be taken from the Qualitative method. Integration is made with: Smooth off, Peak detect Join = 30, Reduce = 50, Raise=5, Draw vertical = 90, detect shoulders = off.

2. Calculate Area% and Norm% values for each peak.

   These values are calculated for each chromatogram separately. The peak data set associated with a specific chromatogram is supplied via the AddData function to any Qualitative Plot control plotting that chromatogram.

3. Combine the peaks from all chromatograms and sort the peaks in retention time order.

   - If more than one peak maximizes within ±2 scans, eliminate all but the one with the largest area, or the first one if there are two with equal area.

   - If 'Exclude target compounds' is set in the method, remove peaks that maximize within ±2 scans of the actual retention time of the target compound taken from the quantification results. This setting is ignored if no quantification results are available. If this option is not checked and quantification results exist then these results (compound name, concentration and concentration units) will be associated with the appropriate peak in the data source. However, Area% and Norm% results will always come from the qualitative processing.

4. Sort in descending area order.

5. Eliminate all but the largest (by area) n peaks (where n is the 'Largest peaks' parameter from the qualitative method).

6. Re-sort in retention time order.

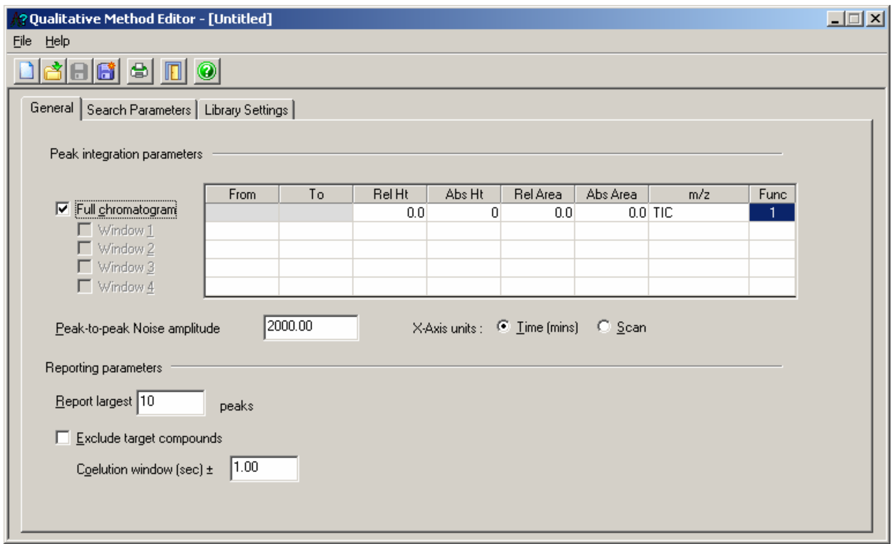
7. Add the peak data to the data source.

Qualitative Method Editor

The main window consists of menu bar, tool bar, and three tabs of parameters.

- General
- Search Parameters
- Library Settings

The General parameters are needed for all qualitative reports that require a peak data set. Since Search Parameters and Library Settings are only required when a library search is to be performed these have been placed on secondary tabs.



Qualitative Method Editor Toolbar

The Toolbar is displayed at the top of the Qualify window. By choosing the toolbar buttons, you can perform some common operations.

 Creates a new qualitative method.

 Opens an existing qualitative method.

 Saves the current qualitative method.

 Saves the qualitative method with a new name.

 Prints the qualitative method.

 Closes the Qualitative Method Editor.

 Displays the help associated with this screen.

Qualitative Method Editor: General Tab

To define parameters for creation of a qualitative peak data set:

- Specify the chromatographic data sets which are to be subject to peak detection and integration. The options are:

  The full chromatogram from start to end

  OR

  One to four segments with specified start and end times.

- Each chromatographic data set can be the TIC, the BPI chromatogram, or a mass chromatogram defined with the usual TurboMass expression.

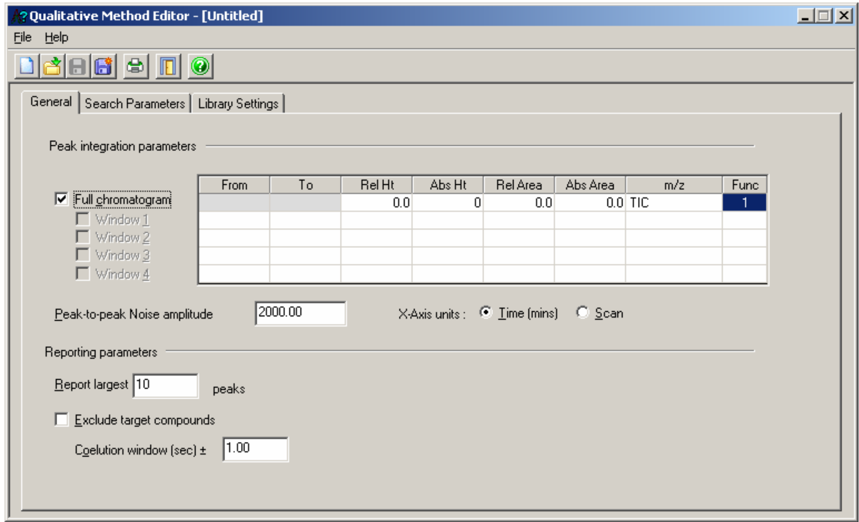
- Define the threshold parameters for each chromatographic data set.

- Define the default peak-to-peak noise amplitude value.

- Set the desired number of peaks to be reported and optionally exclude Quantify target compounds (where applicable).

- Set a ‘coelution window’ parameter to ensure reliable identification of target compounds within the qualitative chromatograms when the Quantify Trace and qualitative peak do not maximize at the identical retention time (default 1 second).

The General Tab Fields



Full chromatogram — Integrate the full chromatogram to create a peak list

Window 1 — Use the first data segment in creating a peak list

Window 2 — Use the second data segment in creating a peak list

Window 3 — Use the third data segment in creating a peak list

Window 4 — Use the fourth data segment in creating a peak list

grid — Defines time segments and integration thresholds. The first two cells in the first edit row (alongside Full Chromatogram) are always disabled and cannot be selected.

Peak–to–peak noise amplitude — Sets the maximum noise expected on the signal

X-Axis units: — Time - Selects Time units for setting the 'From' and 'To' values in the grid.

	Scan - Selects Scan numbers for setting the 'From' and 'To' values in the grid.
Report largest n peaks	The number of peaks to be reported.
Exclude target compounds	Do not include target compounds in the peak list.
Coelution window (sec) ±	Time window for qualitative and Quantify Trace peaks to maximize and still be considered same compound.

Qualitative Method Editor: Search Parameters Tab

To define the criteria for library search operation:

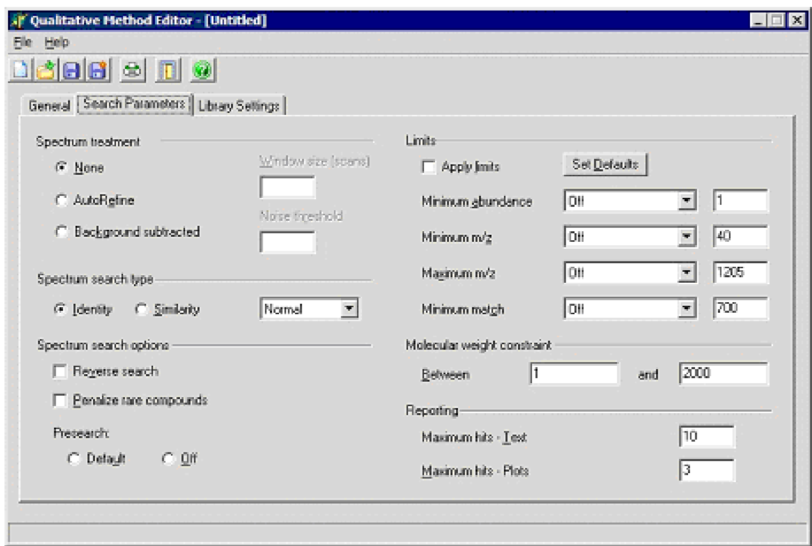
Select the treatment to be applied to the spectrum before initiating the search.

Select the thoroughness of the search (the 'Spectrum search type') and its options. More thorough searches take longer.

Optionally select the 'Reverse search' option to improve the matching capability when there are contaminant peaks in the mass spectrum.

Optionally restrict the mass range of the searched reference spectra if he has some prior knowledge of the compound molecular weight. This will improve matches where the reference spectra may have peaks outside the acquired range.

Optionally restrict the range of the matched compounds, if he has some prior knowledge of the compound molecular weight. This will improve the match quality by only returning results with molecular weights within this range.



The Search Parameter Tab Fields

Spectrum Treatment

None	Use original spectrum scan for search.
AutoRefine	AutoRefine the spectrum prior to search.
Background subtracted	Average the top 3 apex scans, and subtract the scan prior to GC peak start.

The 'Window size' and 'Noise threshold' fields are enabled only when 'AutoRefine' option is selected.

Window size (scans)	Window size parameter for Refine algorithm.
Noise threshold	Noise threshold parameter for Refine algorithm.

Spectrum Search Type

Identity Specifies an Identify type search.

Similarity Specifies an Similarity type search.

<drop–down list> Defines the specific Identify or Similarity search mode.

(Contents of the drop–down list change depending on the selection made with the radio buttons.)

Spectrum Search Options

Reverse search Use Reverse Search scoring

Penalize rare compounds Penalize a match by up to 50 points (out of 1000) depending on how common the compound is.

Default Normal operation, use presearch screening before spectrum-by-spectrum match factor calculation

Off Search the entire database using only the detailed match algorithm

Limits

Apply limits Constrain the possible matches with the selected limits. State of check box does not affect accessibility to other controls in the group.

Set Defaults Set all limits to Default values. (Clicking this button restores the settings in the Limits group to default values.)

Minimum abundance <drop–down list> Determines whether the minimum abundance limit will be used.

<text box> - Smallest peak that will be used in comparison. Used to force small peaks in the target spectrum to be ignored. The value is only enabled when 'Minimum abundance' drop down list is set to 'On'

Minimum m/z <drop–down list> Determines whether or how the minimum m/z limit will be used.

<text box> - Used to determine the lowest m/z used for match factor calculation. Without this specification, the matching algorithm starts comparison at the HIGHER of the minimum m/z values in the target or the library spectra. The value is enabled when 'Minimum m/z' drop–down list is not set to 'Off'

Maximum m/z Determines whether the maximum m/z limit will be used.

<text box> Peaks above the specified mass are ignored. Use to exclude spurious high mass peaks in the search spectrum. The value is only enabled when 'Maximum m/z' drop-down list is set to 'On'.

Minimum match Determines whether the minimum match value will be used.

<text box> - Only compounds with a match value above the entered value will be included in the 'hits' list. The value is only enabled when 'Minimum match' drop-down list is set to 'On'.

Molecular weight constraints

Between	Lower limit for library compound molecular weight.
and	Upper limit for library compound molecular weight. Reporting

Reporting

Maximum hits - Text	The maximum number of hits for which text information will be provided for reporting.
Maximum hits - Plots	The maximum number of hits for which plots will be available for reporting.

Qualitative Method Editor: Library Settings Tab

You may have several mass spectral libraries on your computer. Some are from NIST (mainlib, the main library, and replib, a smaller library of replicate spectra (same compounds, different spectra) which can improve the chances of finding the right compound. There can also be other commercial libraries (e.g. the Pfleger-Mauer-Weber drug library) or user-created libraries.

This tab allows you to select which libraries to search, and in what order. Restricting the number of libraries (spectra) searched increases speed in a linear fashion. Searching libraries which have only the target compounds with few "unlikely" matches also increases the chance of a correct match. For example, someone doing drug analyses might search a drug library, but would not want to search a flavors and fragrances one.

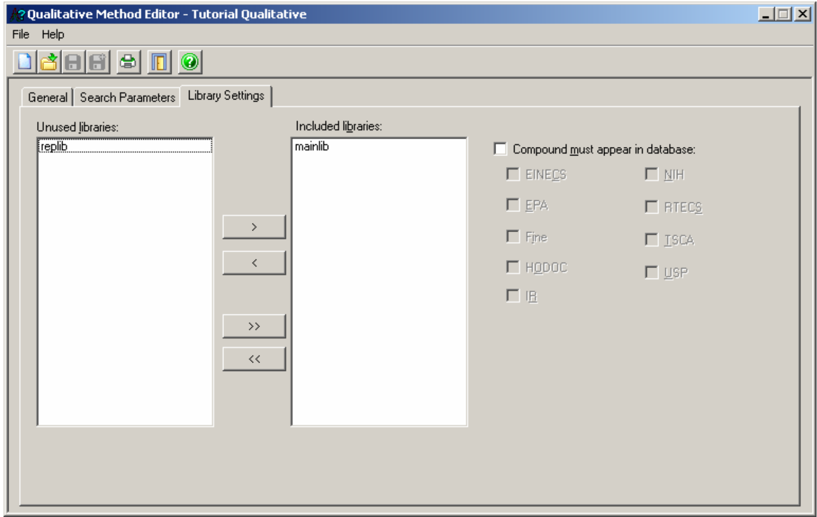
Compounds in mainlib (the primary NIST library) have flags indicating which databases they originally came from or in which industry-standard lists of compounds they occur. If the unknown compound is expected to be in one of these databases or lists, the speed and accuracy of the search can be improved by restricting results to members of those databases or lists.

About NIST Results

- The names in the Qualitative Results may come from the Library Search results, or the Quantify results (if they exist).
- If a peak has both Qualitative and Quantify results, the Quantify name is used.
- NIST Library Search results are in upper case, Quantify can have upper or lower.
- NIST results should use the fonts "NIST Serif" or "NIST Sans Serif" to permit display of Greek letters.

NOTE: *To prevent library searching during Qualitative Calculations, make sure the Included libraries field is empty.*

The Library Settings Tab



Unused/Included libraries

Unused libraries	Libraries not being searched. The order in which items appear in the ‘Unused libraries’ list is alphabetical order.
Included libraries	Libraries being searched. The order in which items appear in the ‘Included libraries’ list is the order in which they were moved over (i.e. new items are appended to the list).
>	Search selected libraries
<	Do not search selected libraries
>>	Search all libraries
<<	Remove all libraries from search list

Compound must appear in database

A list of other databases that the compound must be in. The list is processed as a logical OR, that is if 5 of the databases are checked, the compound is found if it is either of the five databases. All of these are only enabled when 'Compound must appear in database' is checked. These states are remembered from the last setting.

EINECS	European Index of Commercial Chemical Substances
EPA	US EPA Environmental Monitoring Methods Index
Fine	Commercially Available Fine Chemical Index
HODOC	CRC Handbook of Data of Organic Compounds
IR	NIST/EPA Gas Phase IR Database.
NIH	NIH–NCI Inventory File
RTECS	Registry of Toxic Effects of Chemical Substances
TSCA	Toxic Substances Control Act Inventory
USP	U. S. Pharmacopoeia/U.S.A.N.

A Step-by-Step Qualitative Method Summary

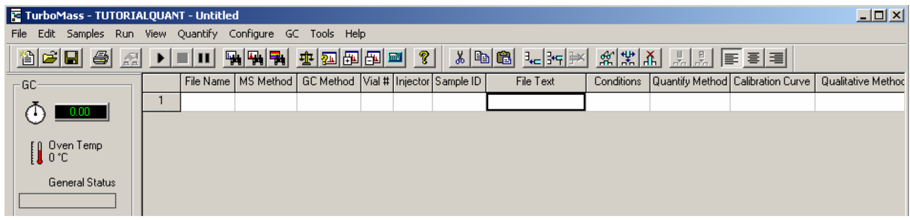
- Create a Sample List
- Create a Qualitative Method
- Put the Qualitative Method in the Sample List
- Start the Analysis

1. Create a Sample List

The first thing that you must do is to create a list of samples that you want to use to perform the analysis. These samples can be acquired manually, but more often they will be acquired automatically using an autosampler. The Sample List Editor has various columns such as Filename, vial or bottle Number and Sample Type that can

be filled in for each sample. Each sample is displayed as one row in the Sample List. The Sample List Editor is part of the TurboMass top-level menu.

You need to tell TurboMass everything that it needs to know about the samples in the list in order for it to perform a complete analysis. You must describe to the system what each of the vials in the autosampler contains, i.e., whether it contains a standard, an analyte, a blank or a QC sample, how to acquire it, its concentration(s), if it is a standard or has internal standards. In addition, you must specify the name of the file in which to store the data. You may also want to add some management information such as Sample ID, the submitter's name, or a sample description, and the Report Method template used.



For more information on how to create a Sample List, see Creating and Editing Sample Lists on page 211.

2. Create a Qualitative Method

A Qualitative Method is required for most Communiqué reporting (an exception is when you just report the chromatogram plot or acquisition conditions).

NOTE*:* *The Quantify Method is required for Calibration and Quantification curves.*

The Qualitative method describes how a data file is processed to produce calibration curves and qualitative information. Details must be entered into the method for each of the compounds being used in the analysis. The Qualitative Method specifies information for performing the following tasks:

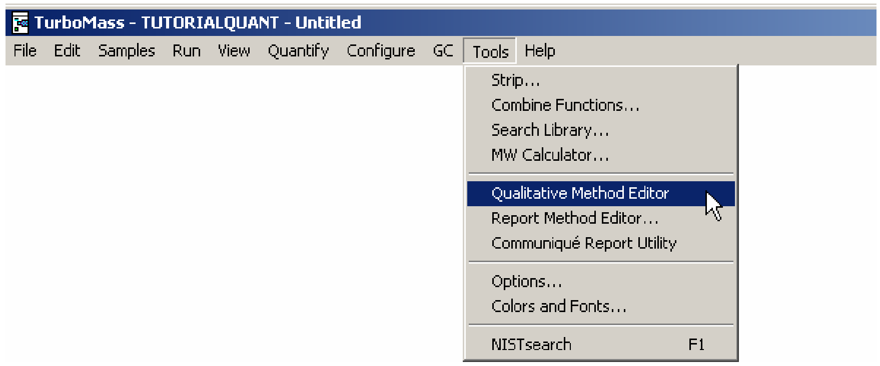
1. Qualitative Peak integration and Reporting parameters.

2. Library Search parameters (Spectrum treatment, search type, search options and limits; molecular weight constraints; and reporting parameters).

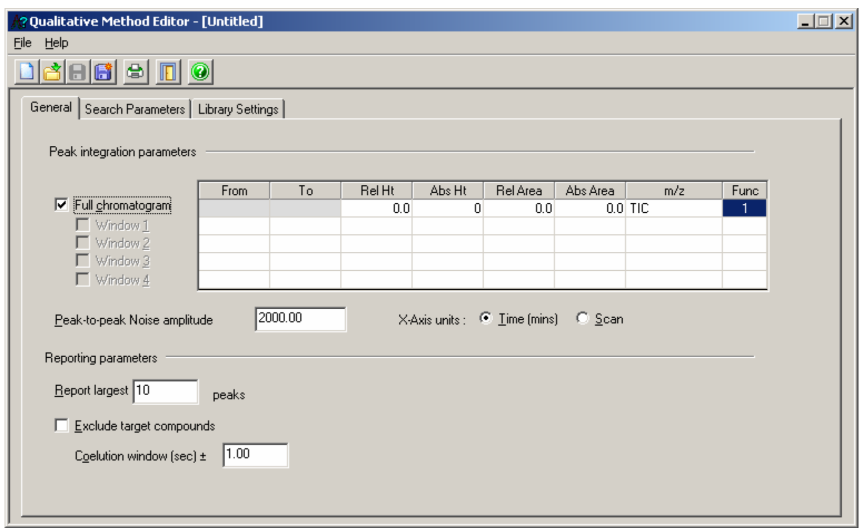
3. Library Selections.

To create a Qualitative Method, follow this procedure:

1. Select **Qualitative Method Editor** from the *Tools* menu



The *Qualitative Method Editor* appears:



The **General** parameters are needed for all qualitative reports that require a peak data set. Since **Search Parameters** and **Library Settings** are only required when a library search is to be performed, these have been placed on secondary tabs.

2. Specify the chromatographic data sets which are to be subject to peak detection and integration.

   The options are: The full chromatogram **From** start **To** end.

   OR

   One to four segments (**Windows 1-4**) with specified start and end times.

NOTE*: Enter the peak integration parameters in the same manner as you have done in Chromatogram or Quantify.*

3. Enter a **From** value. A blank cell indicates the chromatogram segment will start from the beginning of the data. The **From** value must be less than the **To** value (unless either is blank).

4. Enter a **To** value. A blank cell indicates the chromatogram segment will end at the end of the data. The **To** value must be greater than the **From** value (unless either is blank).

5. Enter a Relative height threshold (**Rel Ht**) of the peak in the chromatogram. (default is 0).

6. Enter an Absolute height threshold (**Abs Ht**) of the peak in the chromatogram (default is 0).

7. Enter a Relative area threshold (**Rel Area**) of the peak in the chromatogram (default is 0.0).

8. Enter an Absolute area threshold (**Abs Area**) of the peak in the chromatogram (default is 0.0).

9. Enter a mass **(m/z)**or mass function (**Func**) for the segment (enter TIC, a selected ion, or a valid mass chromatogram equation).

10. Enter the **Peak-to-peak Noise amplitude** value for integration.

11. Select the **X-Axis units Time (min)** or **Scan**.

    Time - Selects Time units for setting the 'From' and 'To' values in the grid.

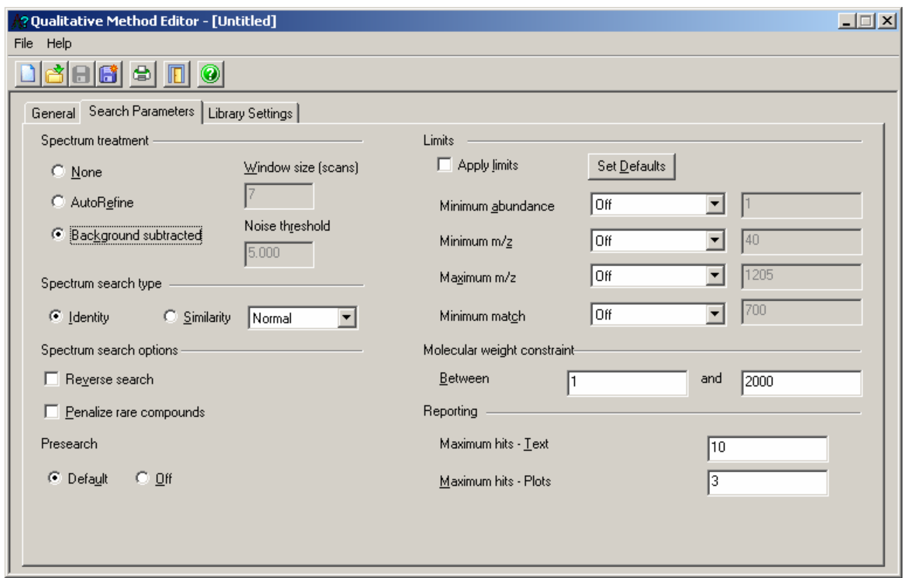
    Scan - Selects Scan numbers for setting the 'From' and 'To' values in the grid.

12. Enter the number of largest peaks you want to report.

13. Set a 'coelution window' parameter to ensure reliable identification of target compounds within the qualitative chromatograms.

    Peaks identified in the quantitative results can be missed in the qualitative report if their retentions do not exactly match those found by the qualitative report method. This can occur because two specific masses in a peak may maximize one or two scans away from each other (of the TIC) due to noise and scan-rate induced 'spectral skewing".

14. Click on the Search Parameters tab.



15. Select the **Spectrum Treatment** to be applied to the spectrum before initiating the search. For example, **Background Subtracted**.

16. Select the thoroughness of the search (the **Spectrum search type**) and its options. Keep in mind that more thorough searches take longer.

17. You can select the **Reverse search** option to improve the matching capability when there are contaminant peaks in the mass spectrum.

18. You can leave the rest of the settings as their default values or optimize as needed.

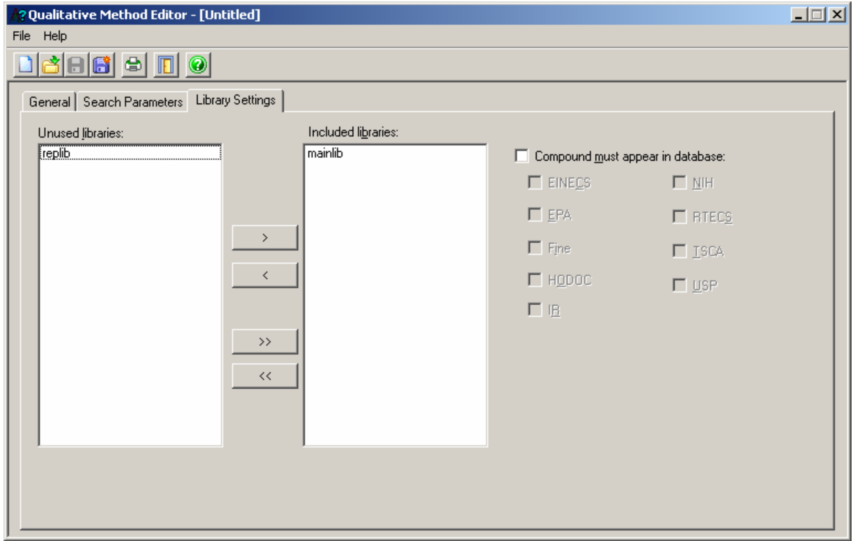
19. Click the **Library Settings** tab.

    You may have several mass spectral libraries on your computer. Some are from NIST (mainlib, the main library, and replib, a smaller library of replicate spectra (subset of compounds, different spectra) which can improve the chances of finding the right compound (Refer to the NIST2002 Software Manual on the NIST2002 CD). There can also be other commercial libraries (e.g., the Pfleger-Mauer-Weber drug library) or user-created libraries.

    This tab allows you to select which libraries to search, and in what order. Restricting the number of libraries (spectra) searched increases speed in a linear fashion. Searching libraries which have only the target compounds with few "unlikely" matches also increases the chance of a correct match. For example, someone doing drug analyses might search a drug library, but would not want to search a flavors and fragrances one.

    Compounds in mainlib (the primary NIST library) have flags indicating which databases they originally came from or in which industry-standard lists of compounds they occur. If the unknown compound is expected to be in one of these databases or lists, the speed and accuracy of the search can be improved by restricting results to members of those databases or lists.

NOTE: *If no libraries are selected, no library search will be performed. This is the default method for only picking Qualitative Peaks.*



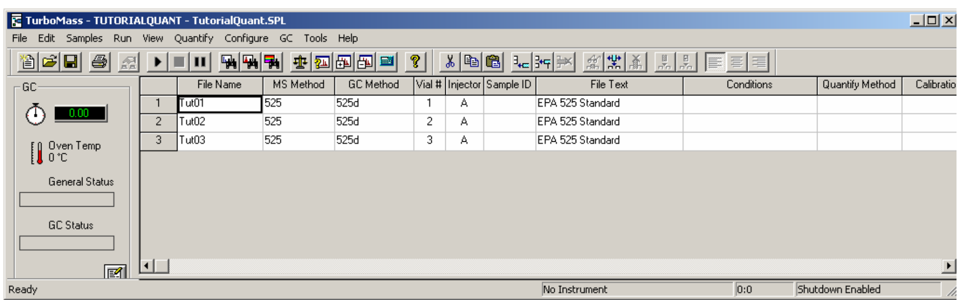
20. Click **Save** or **Save As** from the File menu, then name and save the method.

    This method name will now be available in the **Sample List** under the **Qualitative Method** column.

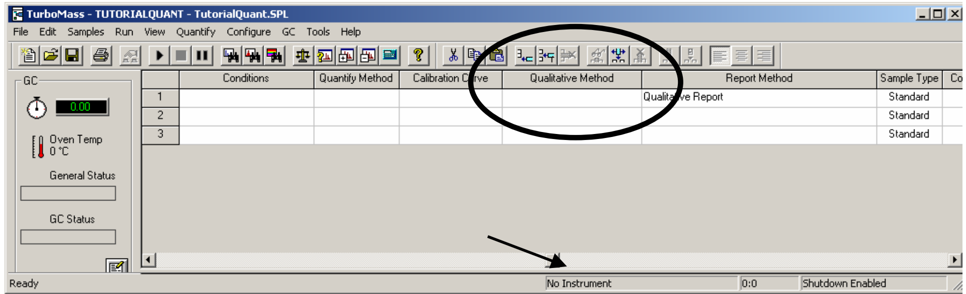
3. Put the Qualitative Method in the Sample List

After creating and saving a Qualitative Method, enter it in your Sample List.

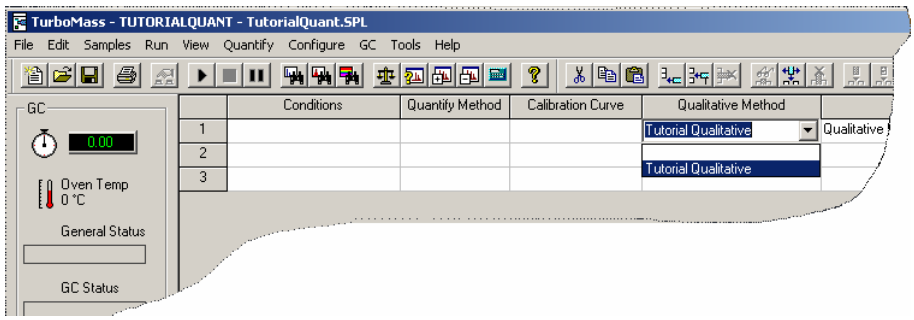
1. Display your **Sample List**.



2. Move the slider on the bottom of the Sample List window to the right until you can view the **Qualitative Method** column.



3. Double-click in the cell and select your **Qualitative Method**.



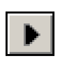
4. Start the Analysis

Before starting an analysis save any changes made to the Sample List by selecting **Save** or **Save As** from the Sample List *File* menu.

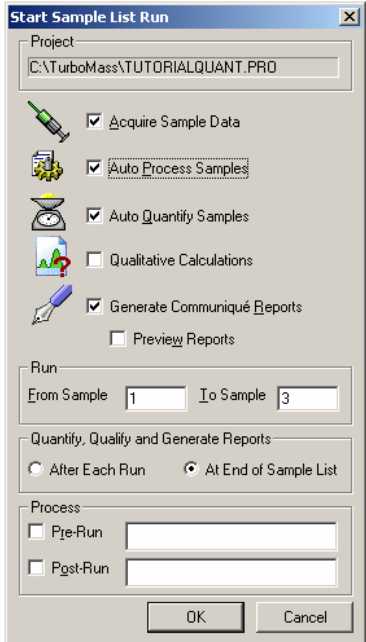
To begin acquiring data or perform post-run reporting:

1. Choose **Start** from the TurboMass top-level *Run* menu

OR-

Choose  to open the Start Sample List Run dialog box.

The Start Sample List Run dialog appears:



2. Enter values or check boxes in this dialog. (The order in this dialog indicated the order of execution. For Example, you **Acquire Sample Data**, then **Auto Process Samples**, **Auto Quantify Samples**, perform **Qualitative Calculations**, and **Generate Communiqué Reports**.)

   Project - The name of the current project appears in this text box. To acquire data to a different project, choose OK or Cancel exit this dialog box, open another project, and restart data acquisition.

   Acquire Sample Data - Selecting this option will acquire data for the specified samples in the list.

   Auto Process Samples - Selecting this option will process the acquired data as specified in the Process column of the Sample List.

   Auto Quantify Samples - Selecting this option will automatically enable sample quantification..

Qualitative Calculations - Selecting this option will enable Qualitative Method processing

Generate Communiqué Reports - Selecting this option will enable Communiqué Report generation.

Preview Reports - Check this box to specify that the Communiqué reports generated during processing will be displayed in a preview window prior to printing (or saving to a file or database).

NOTE: *The five options above allow you to acquire and immediately process and quantify data as desired. Or, you may choose to process or quantify data at a later time.*

Run: From Sample n To Sample m - Sets the range of samples in the sample list which will be acquired/and or analyzed. If you highlight a range of rows before starting the analysis, the first and last rows of the highlighted region will be displayed here.

Quantify, Qualify and Generate Reports: After Each Run - Indicates specified processing will occur after each row in the Sample List.

At End of Sample List - Indicates specified processing will occur only after the sample list is complete.

Process: Pre-Run - Specify the name of the process that will be run before the acquisition of the files in the Sample List.

Post-Run - Specify the name of the process that will be run after the acquisition of the files in the Sample List. For example, to switch the instrument out of the operate mode and turn off various gases.

NOTE: *If you want to run a process after each sample in the Sample List has been acquired, format the Sample List to display Process and enter the name of the process to be run for each of the samples. If you want the process to automatically operate on the data file that has just been acquired, select Options from the Sample List Tools menu, then deselect the Use Acquired File as Default parameter on the System tab.*

3. When all are entered, click **OK**.

Data Acquisition 12

Starting an Acquisition

There are two ways of starting an acquisition, a single sample acquisition from the Tune page or a multiple sample one from the TurboMass top level screen.

Single Sample

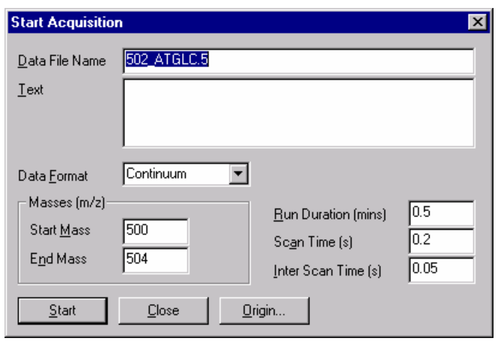
Starting a single sample acquisition

1. Click **Acquire** on the Tune page.

2. Set the required parameters.

3. Click **Start** to begin data acquisition.

   Note that this method of starting an acquisition does not have a solvent delay time or specify a GC method. It is best for recording background and calibration gas spectra.



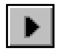
Multiple Samples

The TurboMass top level window contains a Sample List Editor for defining multiple (one or more) samples that may be used together to perform a quantitative analysis. The list of samples is set up using the spreadsheet style editor, which can be tailored to suit different requirements.

Starting a multi-sample acquisition

1. Set up a Sample List as described on page 205.
2. Select **Start** from the **Sample List Run** menu

   OR

   Click  to display the Start Sample List Run dialog.

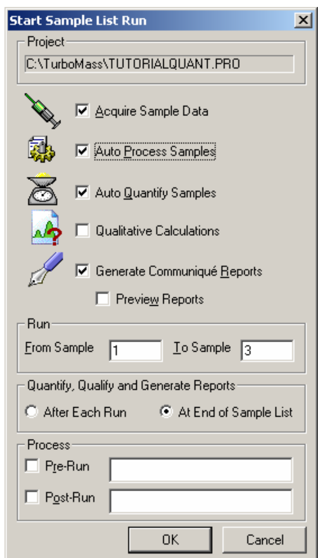
3. Select the **Acquire Sample Data** checkbox.

   Select **Auto Process Samples** to automatically process data with macros once it has been acquired. Select **Auto Quantify Samples** to automatically perform quantification at the end of the sample list.

4. Enter values in the **Run From Sample** and **To Sample** fields.

   The default is all samples in the list.

5. Click **OK**.



6. Repeat steps 1 to 5 as required. Sample Lists will be added to a queue and will run sequentially.

7. The sample in the Sample List that is currently being acquired will have a green next to it.

NOTE: *Filenames in a Sample List must not be duplicated, and Sample List names in a queue must not be repeated.*

Process The Process parameters allow you run processes before and after the Sample List.

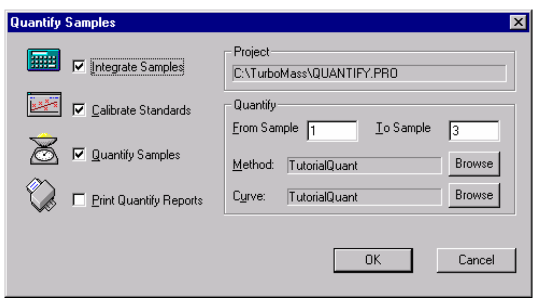
Pre-Run Specify the name of a process that will be run before acquisition of the files in the sample list.

Post-Run Specify the name of a process that will be run after acquisition of the files in the sample list, for example, to switch the instrument out of the operate mode and to turn off various gases.

If you want to run a process after each sample in the sample list has been acquired, format the Sample List to display **Process** and enter the name of the process to be run for each of the samples. If you want the process to automatically operate on the data file that has just been acquired, select **Options** from the Sample List **Tools** menu, then deselect the **Use Acquired File** as Default parameter on the **System** tab.

Automated Analysis of Sample List

1. Select **Process Samples** from the **Quantify** menu to display the Quantify Samples dialog.
2. Select the checkboxes required and click **OK**.



The Quantify Samples dialog allows you to automatically process data files once they have been acquired. To integrate samples, calibrate standards, quantify samples, and print quantification reports, select the appropriate checkboxes. For more information on automated sample list analysis refer to *Quantify* on page 247.

Integrate Samples	Integrates all the sample data files named in the Sample List.
Calibrate Standards	Uses integration results to form Quantify calibration curves.
Quantify Samples	Uses integration results and Quantify calibration curves to calculate compound concentrations.
Print Quantify Reports	Prints the results of integration and quantification.
Project	Displays the project into which data will be acquired. If you want to change the project into which data will be acquired, you can cancel the acquisition and create a new project by selecting **Project Wizard**, or open an existing one by selecting **Open Project** from the Sample List **File** menu. Note that this means that data may only be processed from one Project at a time. Make sure that all data files you might want to process at the same time are acquired to the same Project.
Quantify From Sample n To Sample n	Sets the range of samples in the Sample List that will be analyzed.

Monitoring an Acquisition

Acquisition status is shown on the TurboMass top level display.

GC Status

If GC control is configured, the GC run time is shown on the GC panel along with the oven temperature, General Status, and GC Status.

General Status refers to the PC communications with the GC while GC Status refers to the state of the GC, usually with respect to the current run. Both are described in *GC Control* on page 139.

The scan status, sample number, and scan number are shown in the Status bar at the bottom of the window.

MS Status

If a GC is not configured, the MS run time is shown on the MS panel, and the scan status, sample number, and scan number are shown on the Status bar at the bottom of the window.

The MS status displays several states:

State	Color	Meaning
Operate	Green	High voltages are on, data acquisition is possible
	Red	High voltages are off, data acquisition is not possible
Pressures	Green	High vacuum pump is up to speed
	Red	High vacuum pump is not up to speed

Filament	Green	Operate is on, filament is on
	Red	Operate is off, filament is off - possible open filament

Chromatogram Real-time Update

To view the chromatogram that is currently being acquired in real time:

➢ In the Chromatogram window, click 

OR

Select **Real-Time Update** from the **Display** menu.

The chromatogram display will be updated as the acquisition proceeds.

Spectrum Real-time Update

To view the spectrum that is currently being acquired in real time:

1. Open the data file from the Chromatogram window

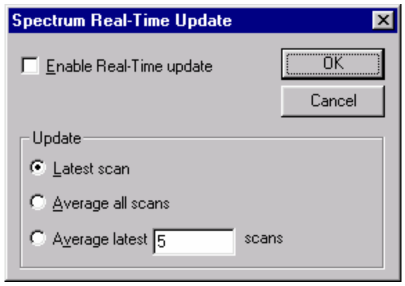
   OR

   Use the TurboMass Data Browser.

2. In the Spectrum window, click 

   OR

   Select **Real-Time Update** from the **Display** menu.



To turn on Real-Time Update, select **Enable Real-Time update**; to turn it off, deselect **Enable Real-Time update**. When Real-Time Update is turned on, the display will continually be updated with spectra from the current acquisition. The actual information displayed is determined by selecting one of the options. Real-Time Update can also be turned on and off by clicking the Real-Time spectrum toolbar button.

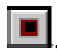
Latest scan	Displays the last acquired scan. This is the default option.
Average all scans	Updates the display with spectra formed by averaging all the spectra that have so far been acquired.
Average latest scans	Updates the display with spectra formed by averaging the last *n* scans acquired, where *n* is specified in the associated field.

Stopping an Acquisition

To stop an acquisition, do one of the following:

- From the Tune page, click .
- From the TurboMass top level window, select **Stop** from the **Run** menu

  OR

  Click .

Data acquired up to this point will be saved.

TurboMass will ask whether you want to stop the GC as well. Respond appropriately.

If you stop the GC, you will need to select **Retry Injection** from the top level **GC** menu to restart the GC.

For more information on starting and stopping the GC, see *Stopping and Restarting the GC* on page 179.

Automatic Startup

TurboMass includes a Startup facility that can be used to startup an instrument to perform an acquisition. Startup can be used in any ionization mode.

The Startup facility will do the following:

- Switch the instrument into Operate mode.
- Load the Tune page and the startup Tune parameters.
- Turn off Operate at the end of the Sample List and shut off the CI gas.

Running Startup

Startup uses the current Tune page settings. To change these settings, open a new file on the Tune page. Startup can be run in any of the following ways:

- Select Startup from the TurboMass **Run** menu.
- Start an acquisition from the Tune page.
- Start a Sample List run.
- In the Sample List **Run** menu, select **Edit Shutdown**. In the Shutdown dialog, select **Startup** from the **Control List** menu.

Automatic Shutdown

TurboMass includes a Shutdown facility that can be used to shut down the mass spectrometer at the end of a Sample List. Shutdown can be used in any ionization mode.

The Shutdown process will do the following:

- Switch the instrument to Standby mode.
- Open the appropriate Autoshutdown Tune file and apply the shutdown parameters.
- Wait for a user-specified delay time.

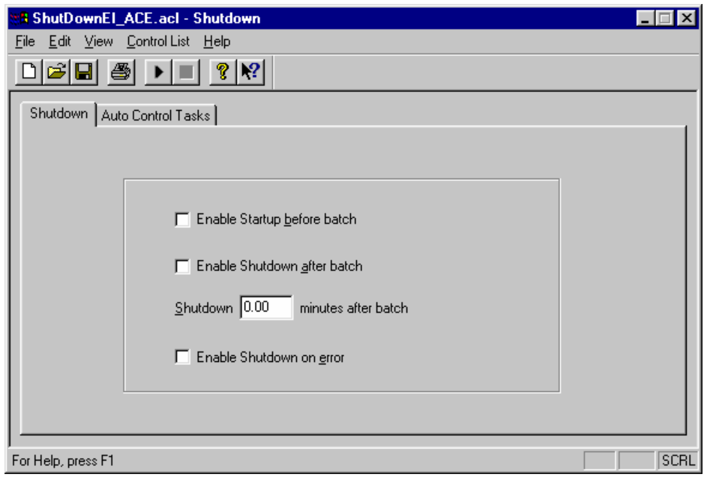
Running Shutdown

Shutdown can be run in either of the following ways:

- Select **Shutdown** from the TurboMass **Run** menu.
- In the Sample List **Run** menu, select **Edit Shutdown**. In the Shutdown dialog, select **Shutdown** from the **Control List** menu.

Editing the Shutdown parameters

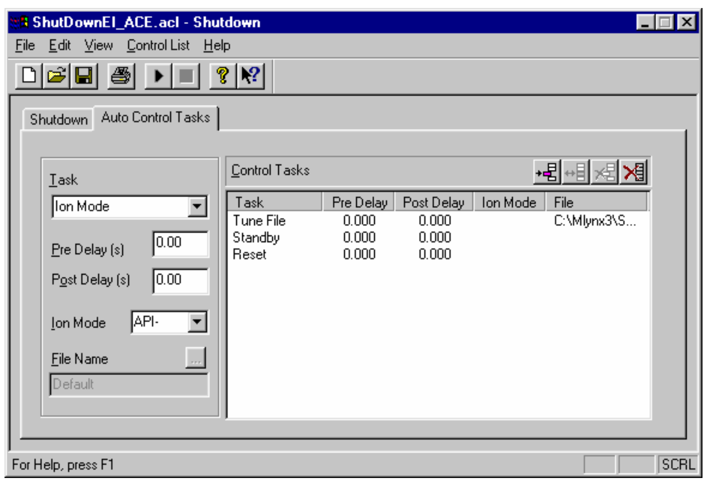
1. Select **Edit Shutdown** from the TurboMass **Run** menu to display the Edit Shutdown dialog.



2. Select the appropriate checkboxes to enable startup before and/or shutdown after a batch run, or on error. Enter the time in minutes when shutdown should start after a Sample List batch run.

NOTE: *Selecting a shutdown time that is too short could cause premature shutdown.*

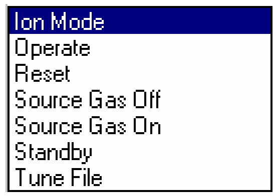
3. Set up an Auto Control Task timetable.



NOTE: *The original parameters are carefully selected. Be cautious about changing them.*

Task

A drop-down list of all the tasks that can be controlled from this page. The list of Tasks will vary depending on the system configuration.



Pre Delay

Time in seconds to wait before this task is run.

Post Delay

Time in seconds to wait after this task is run.

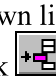
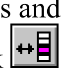
Ion Mode

A drop-down list of Ionization modes. Enabled when **Ion Mode** is selected from the **Task** list.

File Name

Enabled when **Tune File** is selected from the **Task** list. Click  to display the Open file browser and select the required Tune file.

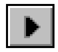
Control Tasks

- To add a Task, select a **Task** from the drop-down list, enter a **Pre Delay** or **Post Delay** time and click .
- To delete a single Task, left-click on the Task in the timetable and click .
- To delete all entries, click .
- To modify a Task, select the required entry in the timetable. The values will then be displayed in the edit fields and can be altered as appropriate. Once changed, click  to modify the values in the timetable.

Running the Auto Control tasks

- Select **Run List** from the **Control List** menu

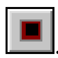
  OR

  Click .

Stopping the Auto Control tasks

- Select **Stop List** from the **Control List** menu

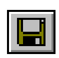
  OR

  Click .

Saving and Restoring Auto Control Task Lists

- To save the settings, select **Save** or **Save As** from the **File** menu

  OR

  Click  and enter a file name in the dialog displayed.

- To restore settings, select **Open** from the **File** menu

  OR

  Click  and select the required file.

Chromatogram 13

Getting Started

Chromatograms are displayed in the TurboMass Chromatogram window.

Displaying the Total Ion Current (TIC) chromatogram

➢ Select **Chromatogram** from the TurboMass **View** menu.

OR

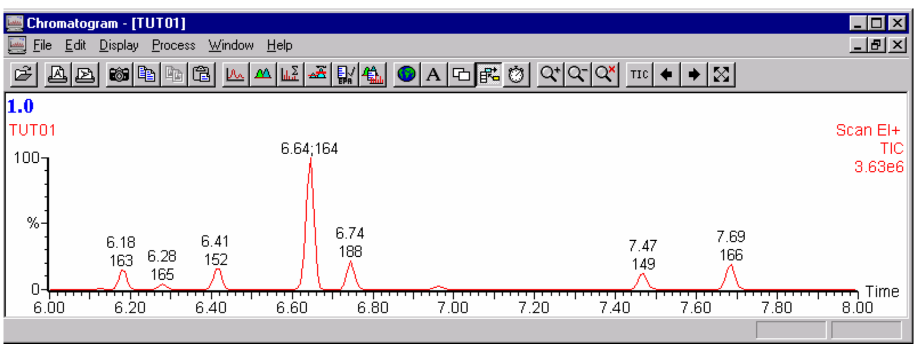
Click .

Displaying a summed mass chromatogram around a peak in a spectrum

➢ Select a peak in a spectrum to display the summed mass chromatogram centered around the selected peak and 1Da wide.

OR

Click  to display the Mass Chromatogram dialog. Enter the mass required in the **Description** field, and click **OK**.



The Chromatogram Display

The chromatogram application runs in a window that has a menu bar at the top. Under each of the headings on the menu bar is a pull-down menu, and every feature of the chromatogram application can be accessed from this menu structure.

At the top of the chromatogram window is the toolbar. The toolbar provides a quick way of performing common operations.

The top level window may contain one or more chromatogram windows, and each can contain one or more chromatogram traces.

The current chromatogram window is identified by having a colored title bar. To select another window to be the current one, either left-click on any part of the new window, or select one from the bottom section of the **Window** menu.

When there is more than one trace in a window, the current one is identified by a colored square to the left of the trace. To select another trace to be the current one, left-click on any part of the trace, select a trace from the **Traces** option on the Chromatogram **Display** menu, or use the up and down arrow keys on the keyboard.

The chromatograms in each chromatogram window share a common time axis. To display chromatograms on different time axes, you must put them in separate windows.

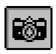
The Chromatogram Toolbar

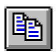
The toolbar is displayed at the top of the chromatogram window and allows you to perform some common operations by clicking the appropriate toolbar button. The default Chromatogram toolbar contains the buttons listed below. It is also possible to customize the toolbar and add additional buttons for other Chromatogram operations.

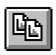
 Opens a data file.

 Prints the current window in portrait format.

 Prints the current window in landscape format.

 Sends a picture of current window to the Clipboard.

 Copies a list of points in the chromatogram to the Clipboard.

 Copies a list of detected peaks to the Clipboard.

 Pastes the contents of the Clipboard onto the display.

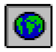
 Selects a mass chromatogram.

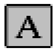
 Performs peak integration.

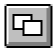
 Combines spectra scans across a chromatogram peak.

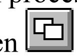
 Compares BFB and DFTPP spectra to US EPA method criteria.

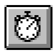
 Performs automatic library searches.

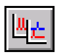
 Select to process all traces in the current window.

 Writes text onto a chromatogram.

 Toggle to display each subsequent chromatogram or chromatogram process in a new window, or to add to the current one.

 Click to cause each subsequent chromatogram or chromatogram process to replace the currently selected trace. Note that  is unavailable when  is chosen.

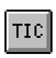
 Toggles real-time chromatogram update on and off.

 Switches between overlay and non-overlay mode.

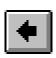
 Increases the magnification of the current range.

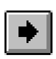
 Decreases the magnification of the current range.

 Deletes the current magnification range.



Resets the display to a TIC trace.

 Decrements the currently displayed scan in the spectrum window.

 Increments the currently displayed scan in the spectrum window.

 Toggle between the previous display range and the default display range.

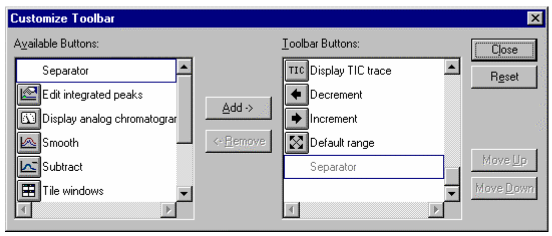
Customizing the Chromatogram Toolbar

The Chromatogram toolbar can be customized to:

- Add other buttons for the operations that you use most frequently.
- Remove buttons you do not require.
- Determine the order in which the toolbar buttons are displayed.

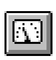
Customizing the Chromatogram toolbar

➢ Select **Customize Toolbar** from the Chromatogram **Display** menu, and add or remove buttons as appropriate.



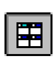
The additional buttons that can be added to the default Chromatogram toolbar are:

 Edit integrated peaks.

 Display analog chromatograms.

 Smooth.

 Subtract.

 Tile windows.

 Cascade windows.

 Stack windows.

Adding buttons to the toolbar

1. In the **Available Buttons** list, select the button you want to add
2. In the **Toolbar Buttons** list, select the toolbar button before which you want to insert the new button.
3. Click **Add** to add the new button.
   Steps 1 to 3 can be repeated as often as required.
4. Separators can be inserted between toolbar buttons to divide them into logical groups. To add a separator, repeat steps 1 to 3 selecting **Separator** in the **Available Buttons** list.
5. Click **Close** to exit and save changes.

Removing buttons from the toolbar

1. In the **Toolbar Buttons** list, select the button you want to remove.
2. Click **Remove** to remove the button.
   Steps 1 and 2 can be repeated as often as required.
3. Click **Close** to exit and save changes.

Changing the order in which toolbar buttons are displayed

1. In the **Toolbar Buttons** list, select the button you want to move.
2. Click **Move Up** or **Move Down** to move the toolbar button.
   Steps 1 and 2 can be repeated as often as required.
3. Click **Close** to exit and save changes.

Resetting the toolbar to default settings

1. Click **Reset**.

2. Click **Close** to exit and save changes.

Displaying/hiding the toolbar in the Chromatogram display

- Select **Toolbar** from the Chromatogram **Display** menu to display/hide the toolbar in the display. This command is a toggle. A check mark will appear next to this menu item when it has been selected.

Displaying Chromatograms

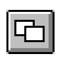
You can display various types of chromatograms in the Chromatogram Window: mass chromatograms, TIC, and BPI chromatograms. You can also display chromatograms in several ways.

Adding or Replacing Chromatogram Traces

TurboMass gives you a number of options for displaying any new chromatogram traces. New chromatogram traces can be generated by:

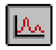
- Opening a new file.
- Processing chromatogram traces (subtract, smooth, integrate, etc.).
- Selecting mass chromatograms with the mouse or by using the Display **Mass** menu command.

To display each new chromatogram trace in a new window, click . To cancel this mode and display new traces in the same window, click  again. When new traces are displayed in the same window, you can choose whether to add the new trace to the traces currently displayed or to replace the current trace with the new trace. Click  to replace the currently selected trace with each subsequent chromatogram or chromatogram process. Click  a second time to add each subsequent chromatogram or chromatogram process to the traces on display. Up to 16 chromatogram traces can be displayed in one window.

NOTE:  *is unavailable when*  *is chosen.*

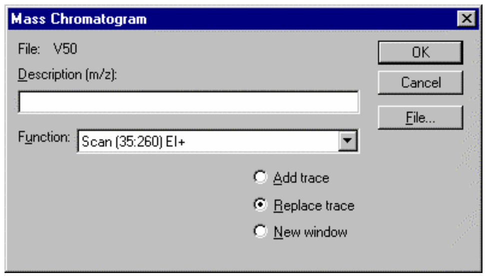
Mass Chromatograms

The following procedure describes how to display a summed mass chromatogram.

1. Click 

   OR

   Select **Mass** from the Chromatogram **Display** menu to open the Mass Chromatogram dialog.



2. If required, select a function from the **Function** drop-down list.

3. Enter the description of the mass chromatogram you want to generate using one of the following formats:

110	The summed chromatogram of masses 109.5 to 110.5
110+340	The summed chromatogram of masses 109.5 to 110.5 and 339.5 to 340.5
110-340	The summed chromatogram of masses 339.5 to 340.5 subtracted from the summed chromatogram of masses 109.5 to 110.5
110_340	The summed chromatogram of all masses from 110 to 340 inclusive

You can generate more than one mass chromatogram trace at a time by separating individual descriptions with commas. For example:

110, 150	The two mass chromatograms centered around 110 and 150
110_150, 340	The summed mass chromatogram of all masses from 110 to 150, and the mass chromatogram centered around 340

4. If you want to add the mass chromatogram to the current chromatogram window, select **Add trace**. If you want the mass chromatogram to replace the currently displayed chromatogram trace, select **Replace trace**. If you want the mass chromatogram to have its own chromatogram window, select **New window**.

5. Click **OK**.

6. Mass Chromatograms can also be generated from a spectrum display. A single right-click on a peak in the spectrum generates a chromatogram centered around the nearest peak. The vertical height at which the mouse is clicked is also taken into account. The peak chosen will be the nearest peak of equal or greater intensity. A right-click-and-drag operation generates a chromatogram for the selected range.

Displaying the same mass chromatograms for a new data file

1. Select **Open** from the Chromatogram **File** menu to load the Chromatogram Data Browser.

2. Select the new data file you want to display.

3. Select **Replace All** to replace the existing data file and also any mass chromatograms that are on display.

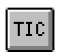
4. Click **OK**.

TIC and BPI Chromatograms

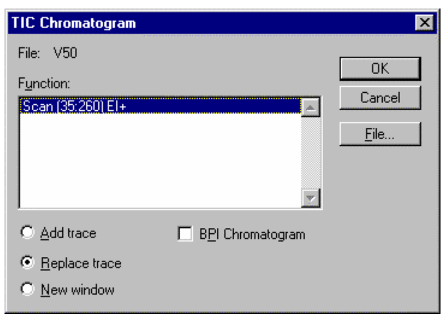
The Total Ion Current (TIC) chromatogram is the default chromatogram displayed when you start the chromatogram module or when you select a new data file using the **File Open** command. The intensity plotted at each point in the TIC is the sum of all the intensities in that scan. You can also obtain the TIC by selecting TIC from the chromatogram toolbar.

A BPI (Base Peak Intensity) Chromatogram plots the greatest intensity at each scan, whereas the TIC is the sum of the noise and the sum of signal at each scan. The BPI chromatogram exhibits a greater apparent resolution and signal-to-noise, but will only contain contributions from the most intense components. Therefore, it is possible that some peaks in the TIC chromatogram may not be visible in the BPI chromatogram. Alternatively, the BPI chromatogram may separate some components that coelute in the TIC.

Displaying a TIC chromatogram using the toolbar

- Click 

to update the Chromatogram display to show a single TIC chromatogram for the currently selected trace.



Displaying a TIC or BPI chromatogram using the menu

1. Select **TIC** from the Chromatogram **Display** menu.

2. If you require a BPI chromatogram, select **BPI Chromatogram**.

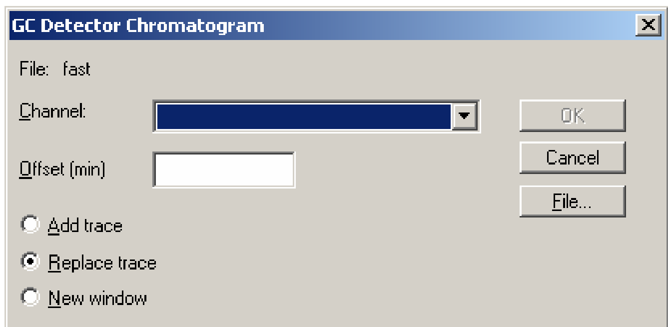
3. If you want to add the new chromatogram to the current chromatogram window, select **Add trace**. If you want the new chromatogram to replace the current trace, select **Replace trace**. If you want the chromatogram to have its own window, select **New window**.

4. Click **OK** to save changes.

GC Detector Trace

This dialog enables you to display the GC chromatograms previously acquired from GC detectors (such as an FID) run in parallel to the MS within the Chromatogram window. You may also specify the GC detector chromatogram as the Quantify Trace for a compound within the TurboMass Quantify Method.

1. Select **GC Detector Trace** from the Chromatogram **Display** menu to open the GC Detector Chromatogram dialog.



Next to File is the name of the currently selected TurboMass raw data file.

Select from the drop–down list the GC detector data channel (A or B) to display.

Enter an Offset (positive or negative) to be applied to the GC detector chromatogram display to help align it with the mass spectrometer chromatogram. For example, a positive offset of 0.15 minutes would cause the plot to start at 0.15 minutes on the time axis. If the X-axis display is changed to 'scans' the previous offset (in minutes) will continue to be used for the GC detector trace.

Select one of the following:

- Add trace: A radio button that indicates the new chromatogram will be added to the current window, in stacked or overlay mode.

- Replace trace: A radio button that indicates the new chromatogram will replace the active chromatogram in the current window.

- New window: A radio button that indicates the new chromatogram will be displayed in a new window.

If necessary, select a new TurboMass raw file by clicking the File button. If a new file is selected the ‘File:’ name displayed will be updated and the ‘Channel’ control will also be updated appropriately.

Aligning GC Detector Traces

Data from the GC detector may be slightly out of phase with data from the mass spectrometer as there may be a time lag between analyte arrival.

You can specify an offset to the time axis of each GC trace to allow you to manually align it with another. A different time offset can be applied to each of the GC detectors acquired. Only the display is affected; the data on disk remain unchanged.

NOTE: *This only works if the horizontal axis is displayed as time and not scans.*

Aligning two chromatograms

1. Select a chromatogram.

2. Select **Align** from the Display/Range dialog.

3. Enter the Offset time that is required to line up the two chromatograms, and click **OK**.

Manipulating the Display

You can alter the displayed ranges of the horizontal and vertical (intensity) axes and set the magnification ranges.

Altering the Horizontal Axis

Do one of the following to alter the range of the horizontal axis.

Altering the range of the horizontal axis (zoom)

- **Use the mouse:** Left-click at one end of the region of interest, and drag the mouse horizontally to the other end. A line appears across the range you have selected. Do not go beyond the bounds of the axis. When you release the mouse, TurboMass redisplays the selected region to fill the current window.

  Repeat this operation as often as required.

- **Use the menu:**
  1. Select **Range From** from the Chromatogram **Display** menu.
  2. Enter new **From** and **To** values for the horizontal axis.
  3. Click **OK**.

Centering the display around a point on the horizontal axis

1. Select either Range, Center, On Scan or Range, Center, On time from the Chromatogram Display menu.

   Only one of these items will be on the menu, depending on the units displayed on the horizontal axis.

2. Specify the scan number or retention time you want to center on.

3. Specify the half-width of the display range in the Window text field.

4. Click **OK**.

Centering the display around a peak list entry

1. Select Range, Center, Peak List Entry from the Chromatogram Display menu.
2. Specify the peak list entry you want to center on.
3. Specify the half-width of the display range in the Window text field.
4. Click **OK**.

Altering the Range of the Intensity Axis

You can alter the range of the intensity axis with the mouse.

- Left-click at one end of the region of interest, and drag the mouse vertically to the other end. A line appears across the range you have selected. Do not go beyond the bounds of the axis. When you release the mouse, TurboMass redisplays the selected range to fill the current window.

  This operation can be repeated as often as required.

Altering the Range of Both Axes

You can alter the range of both axes with the mouse.

- Left-click at one corner of the region of interest, and drag the mouse to the diagonally opposite corner. A box appears around the region you have selected. Do not go beyond the bounds of the axis. When you release the mouse, TurboMass redisplays the selected region to fill the current window.

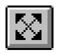
  This operation can be repeated as often as required.

Setting Magnified Ranges

Use the following procedures to set the magnification ranges.

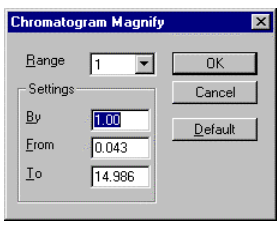
Creating single or multiple magnification ranges

To create single or multiple magnification ranges do any of the following:

- If you have a three-button mouse, middle-click at one end of the region of interest and drag the mouse horizontally to the other end. A line appears across the range you have selected. When the mouse is released, TurboMass redisplays the selected range with an initial magnification factor of 2.
- Hold down the SHIFT key, and left-click and drag the mouse across the region of interest.
- To expand the chromatographic range of interest, left-click and drag the mouse, and click  as many times as required to achieve the desired magnification. Click  to restore the original chromatographic range.
- Set parameters from the Chromatogram **Magnify** menu.

Creating single or multiple magnification ranges using the Magnify menu

1. Select **Magnify** from the Chromatogram **Display Range** menu to open the Chromatogram Magnify dialog.

   OR

   Double-click the magnify range indicators for an existing magnified range.

2. Enter the range to magnify in **From** and **To**. Enter the magnification factor you want to apply in **By**.

3. To define more than one magnification range, select a new range in **Range** and repeat step 2.

   You can define up to five different magnified regions of the chromatogram.

4. Click **OK** to redisplay the chromatogram with the data in the selected region magnified by the requested factor.

   The magnified regions are-displayed in a different color and labeled with the magnification factor.

Magnifying the range of the intensity axis using the Toolbar

- Click  to increase the magnification of the current range.

  The current magnification factor is multiplied by 1.5 and rounded up to the nearest even number to give the increased magnification factor. If the initial magnification factor is 2, this will give subsequent magnification factors of 4, 6, 10, 16 etc.

- Click  to decrease the magnification of the current range.

  The current magnification factor is divided by 1.5 and rounded down to the nearest even number to give the decreased magnification factor. If the initial magnification factor is 16, this will give subsequent magnification factors of 10, 6, 4 etc.

Changing the magnification of a particular range

- Double-click the magnification description of the magnification range to display the Chromatogram Magnify dialog. Enter the new magnification factor and click **OK** to exit.

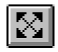
Deleting magnification ranges

1. To delete a single modification range, select the magnification description that appears above the range, and click . The description will change color to red to indicate the currently selected range.

2. To delete all magnification ranges, select **Magnify** from the Chromatogram **Display Range** menu. Click **Default** to delete all magnification ranges.

3. Click **OK** to exit.

Restoring the display

➢ Click  to toggle the display between the previous display range and the default range.

  OR

  Selecting **Default** from the Chromatogram **Display Range** menu toggles the display between the previous display range and the default range.

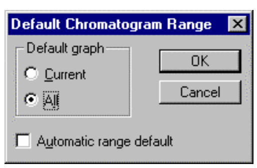
  These operations do not remove magnification ranges.

Setting the Display Range Defaults

The display range default settings specify both the effects of choosing and adding a new chromatogram to the display.

Changing the default display

1. Select **Range, Default** from the Chromatogram **Display** menu.



2. Make any changes.

   Default graph If there is more than one chromatogram in the same window, this option specifies whether the default time/scan range for that window is made large enough to include the time/scan ranges of **All** the chromatograms, or large enough for the **Current** chromatogram only.

Automatic range default If this option is selected, the display range will return to the specified default (see **Default graph**) when a new chromatogram is added to a chromatogram window. If this option is not selected, the display range will remain unchanged when a new chromatogram is added.

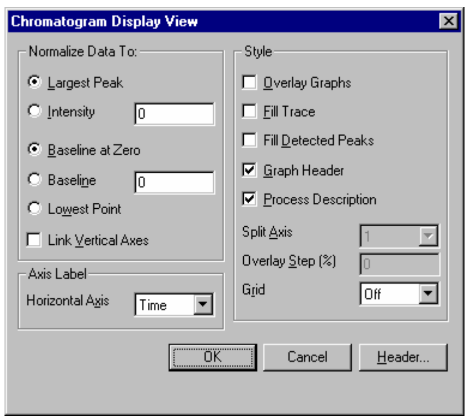
3. Click **OK**.

Controlling the Appearance of the Display

Each chromatogram window has its own set of display parameters that determines the appearance of the chromatogram display. You can inspect and alter the parameters for the current chromatogram window from the Chromatogram Display View dialog.

Changing the display parameters

1. Select **View** from the Chromatogram **Display** menu to open the Chromatogram Display View dialog.



2. Make any changes.

Normalize Data To

These parameters specify the scale on the intensity axis.

Largest If selected, the vertical axis is scaled such that the largest

Peak	peak on the display is at 100 %.
Intensity	If you select **Intensity** and specify a normalizing intensity in the text field, the vertical axis is scaled such that your specified intensity is at 100 %.
Baseline at Zero	If selected, the vertical axis is scaled from 0 %.
Baseline	If you select the **Baseline** parameters and specify an intensity offset in the adjacent text field, the vertical axis is scaled from your specified intensity. This option can be useful for displaying chromatograms that have a raised baseline.
Lowest Point	If selected, the display is automatically scaled such that the lowest point on the trace is at the bottom of the display.
Link Vertical Axes	When comparing two chromatograms by overlaying them, it may be useful to plot both chromatograms on the same intensity scale. The **Link Vertical Axes** parameter allows you to do this. If selected, all axes in the current window will be given a common vertical scale.
Axis Label	The **Horizontal Axis** parameter allows you to specify the units of the horizontal axis to be either time or scans.
Style	
Overlay Graphs	If selected, multiple traces in the same window will be superimposed on the same axis. If not selected, the traces will be drawn on separate axes, arranged vertically. When chromatograms are overlaid, only the currently selected trace is annotated.
Fill Trace	If selected, the area under the chromatogram trace will be colored.
Fill Detected	If selected, then peaks detected by integration are colored.

Peaks

Graph Header The **Graph Header** parameter allows you to turn off the header information normally displayed at the top of the chromatogram, in order to produce data for publication. If selected, the header will be displayed; if not selected, the header will not be displayed.

Process Description Each process performed on a chromatogram adds a summary of its parameters to the chromatogram's header. The **Process Description** parameter allows you to turn off just the process information, and leave the remainder of the header on the chromatogram.

NOTE: *The* **Graph Header** *parameter overrides the* **Process Description** *parameter. That is, if* **Graph Header** *is turned off,* **Process Description** *will be turned off as well.*

Split Axis The **Split Axis** value is enabled when **Overlay Graphs** is selected. It allows you to change the aspect ratio of the chromatogram by dividing the horizontal axis into segments, then arranging the segments vertically. For example, if a chromatogram 30 min in duration is on display, and you set Split Axis to 3, the display will show three axes, one from 0 to 10 min, one from 10 to 20 min, and one from 20 to 30 min.

Overlay Step (%) The **Overlay Step (%)** parameter is turned on when **Overlay Graphs** is selected. It allows you to offset each subsequent chromatogram trace by a percentage of the intensity axis. This can make it easier to examine overlaid traces.

Grid Allows you to fit a grid to the chromatogram display. The pattern of the lines that make up the grid can be chosen as Dot, Dash or Solid.

3. Click **Header** to display the Header Editor where you can edit the header information displayed at the top of the window.

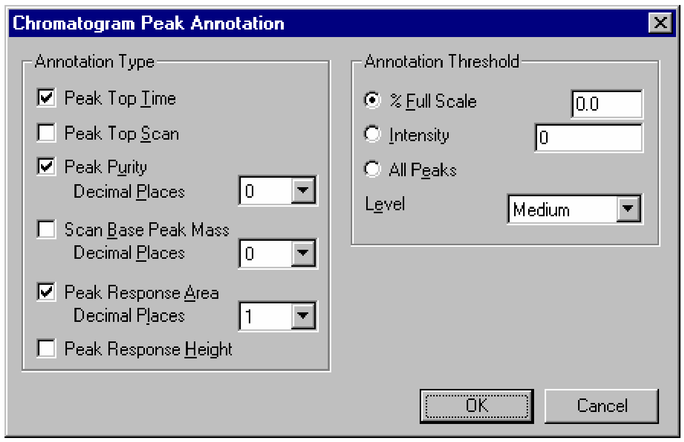
4. Click **OK**.

Controlling the Appearance of Peak Labels

Each chromatogram window has its own set of Peak Annotation parameters, which determine the appearance of peak labels. You can inspect and alter the parameters for the current window from the Chromatogram Peak Annotation dialog.

Changing the peak annotation parameters

1. Select **Peak Annotation** from the Chromatogram **Display** menu to display the Chromatogram Peak Annotation dialog.



2. Make any changes.

3. Click **OK**.

Annotation Type Parameters

These parameters control which types of peak annotation will appear on the chromatogram. The types of peak annotation available are **Peak Top Time**, **Peak Top Scan**, **Peak Purity**, **Scan Base Peak Mass**, **Peak Response Area**, and **Peak Response Height**. To display a particular peak annotation select its checkbox.

For **Scan Base Peak Mass**, you can set the number of decimal places to a value from 0 to 4. For **Peak Response Area** and **Peak Purity** you can set the number of decimal places to a value from 0 to 3. The illustration above shows typical defaults for GC/MS.

If **Display Peak Name** is selected, the peak name, if available, will be displayed above the peak. The Peak Name may be obtained in several ways:

- While viewing Quantification results, double-click on one of the report lines.
- In Chromatogram, integrate the chromatogram. Select **Integrated Peaks** from the **Edit** menu. Select the desired peak and enter the name. Click **Modify** and then **OK**.
- In Chromatogram, display a selected portion of the desired chromatogram (TIC or selection ion). Select **Lib Search Peaks** from the **Process** menu. After the library searching is complete, return to Chromatogram. Select **Integrated Peaks** from the **Edit** menu and click **OK**. This will display the top-match library hits for each of the integrated peaks.

Avoiding Printout of Library Search Results

To avoid printing out extensive library search results, see the following procedure:

1. From the Window **Start** menu, select **Settings > Printers**.
2. In the Printers dialog, double-click on the name of the printer.
3. In the Print Queue dialog, select **Pause Printing** from the **Printer** menu.
4. After library searching is completed, purge the files from the print queue by double-clicking on the printer icon in the Windows task bar, then selecting **Purge Print Documents** from the **Printer** menu. Before closing the dialog, be sure to restart the printer by removing the checkmark from the **Pause Printing** command in the **Printer** menu by selecting the command again.

NOTE: *Pausing the printer pauses it for all users, including others who may access it across a network. If this is a problem, add a new printer in the Printers dialog under*

a custom name and select this printer as your default. Purge the print documents when done as described above.

Annotation Threshold Parameters

Annotation Threshold	Allows you to specify a minimum intensity for a peak to be labeled.
% Full Scale	Allows you to set a threshold as a percentage of the base peak intensity.
Intensity	Allows you to set an absolute intensity threshold
All Peaks	Annotates all peaks, regardless of intensity.
Level	Determines the amount of labels that appear on the chromatogram. The **Level** parameter can be set to **High**, **Medium**, or **Low**.

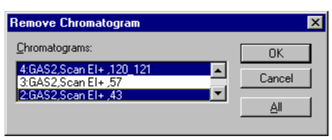
Removing Chromatograms from the Display

You can remove the currently selected chromatogram trace by pressing Delete. A message will ask you to confirm the deletion. Clicking **OK** will remove the trace from the display. This operation does not affect the data stored on disk.

You can also remove traces using the Remove Chromatogram dialog. This is a quicker method if you want to remove more than one trace.

Removing multiple chromatogram traces from the display

1. Select **Remove** from the Chromatogram **Display** menu to display the Remove Chromatogram dialog.



2. The traces in the current window are listed in the order in which they appear on the display. You can select one or more traces in the list. Clicking again on a selected item will cancel the selection. You can select all the traces by clicking **All**, and then clicking **OK**.

Real-time Display of Chromatograms

If you are acquiring data into a file, and displaying chromatograms from that file, then you can watch the chromatogram build up by clicking  or by selecting **Real-Time Update** from the Chromatogram **Display** menu.

Each chromatogram window has a separate real-time update switch. You can see the state of the switch for a particular window by determining if  is selected, or by making that window current and selecting the Chromatogram **Display** menu. If real-time update is enabled, **Real-Time Update** has a check mark by it.

Changing the Order of Displayed Chromatograms

When a window contains multiple traces you can change the order in which they are displayed. The chromatogram that is first in the list being displayed at the bottom of the screen, or on top of the others, if graphs are overlaid.

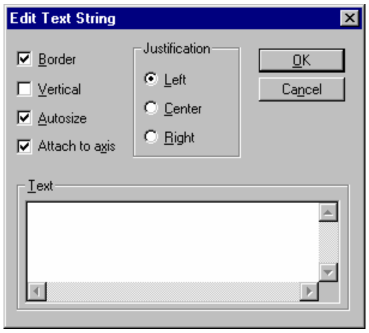
Select **Move To First** from the Chromatogram **Display** menu to display the currently selected chromatogram at the bottom of the screen.

Select **Move To Last** from the Chromatogram **Display** menu to display the currently selected chromatogram at the top of the screen.

Adding Text to the Chromatogram Display

To add text labels to the chromatogram display, click .

When selected, the Text tool button changes color to show that it is active. Position the cursor where you want to add text, and left-click to open the Edit Text String dialog.



Enter the text in the **Text** field, select desired options, and click **OK**. You can change the position of the user text by dragging it to a new position. Use the handles at the sides or corners of the text box to size the box. If you want to edit the text, double-click it to redisplay the Edit Text String dialog.

The font and color of the user text can be changed in the Colors and Fonts option on the TurboMass **Tools** menu. Any changes made to fonts or colors will only apply to text added after the changes. If you want to change existing text, you must delete and reinsert it. Other formatting options available for user text are as follows.

Justification Aligns text to the left, right, or center of the text area.

Border Draws a box around the user text.

Vertical Displays text vertically rather than horizontally.

Autosize Defines the text area to be just large enough to hold the user text. If not selected, use the handles that appear to size the text area as required.

Attach to axis If selected, user text can be positioned only within a box defined by the intensity and time/scan axes. If it not selected, user text can be positioned anywhere on the display.

The current formatting options are saved as the default options each time you exit from the Edit Text String dialog.

Processing Chromatograms

Three processes are available for use on chromatograms: polynomial background subtraction, smoothing, and integration. Background subtraction and smoothing help you improve the presentation of the data. Integration locates peaks, positions baselines, and calculates peak statistics for quantitative work.

Processing Multiple Chromatograms

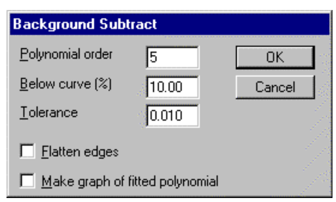
The background subtract, smooth, and integrate processes can be performed automatically on all the chromatograms within the current window. To enable this operation, click or select **Process All Traces** from the Chromatogram **Process** menu; the menu item will have a check next to it. To turn off multiple processing, reselect the toolbar button or menu item.

You can choose to add the processed trace to the current window or replace the current trace with the processed trace. Toggle to cause each subsequent chromatogram or chromatogram process to replace the currently selected trace or to add chromatogram process to be added to the display.

NOTE: *is unavailable when is selected.*

Subtract

Background Subtract fits a smooth curve through the noise in the chromatogram, and then subtracts this curve from the chromatogram, leaving the peaks on a flat baseline.



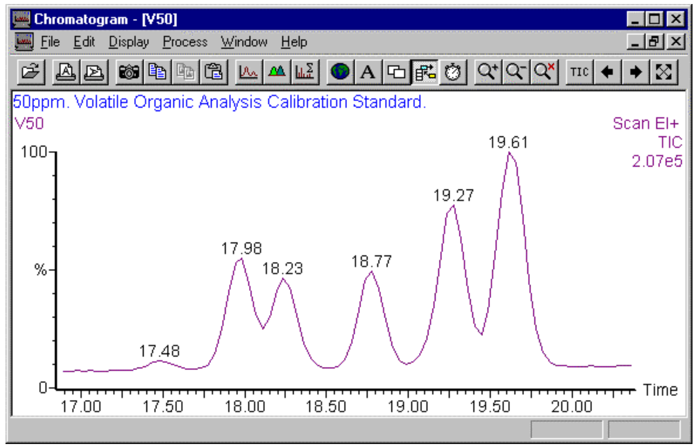
Polynomial Order Allows you to specify the degrees of freedom allowed to the fitted curve. With polynomial order set to 0, a horizontal straight line is fitted. With polynomial order set to 1, a sloping straight line is fitted. The further the background is from a straight line, the higher you must set the Polynomial Order value. Too high a value will cause the fitted curve to begin to follow the peak shapes. Normal operating range for this parameter is 3rd to 20th order.

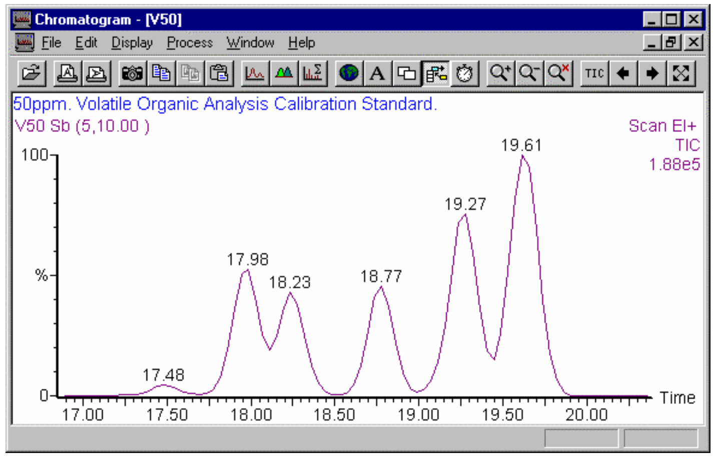
Below Curve Allows you to move the background curve up and down in the noise. The curve fit is constrained to place the specified percentage of data points beneath the fitted background curve. The normal operating range for this parameter is 5 % - 30 %, depending on the abundance and width of peaks in the chromatogram. For more or wider peaks, increase the value.

Tolerance Affects the precision to which the internal arithmetic is performed. It should not normally be changed from its default value of 0.01.

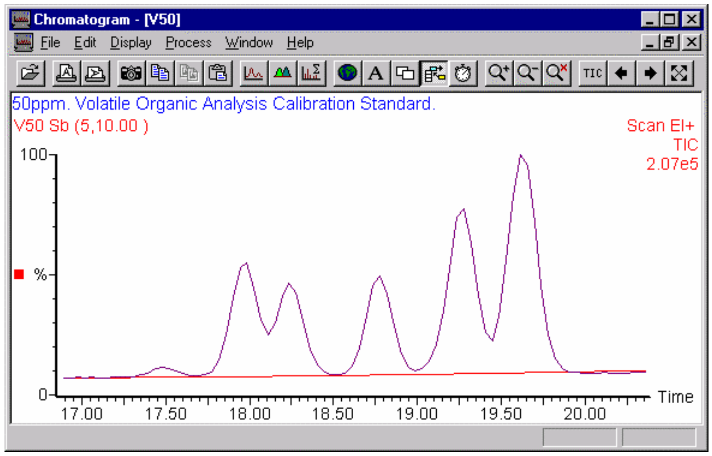
Flatten Edges If selected, TurboMass verifies that the polynomial applied is flat or horizontal at the beginning and end of the trace.

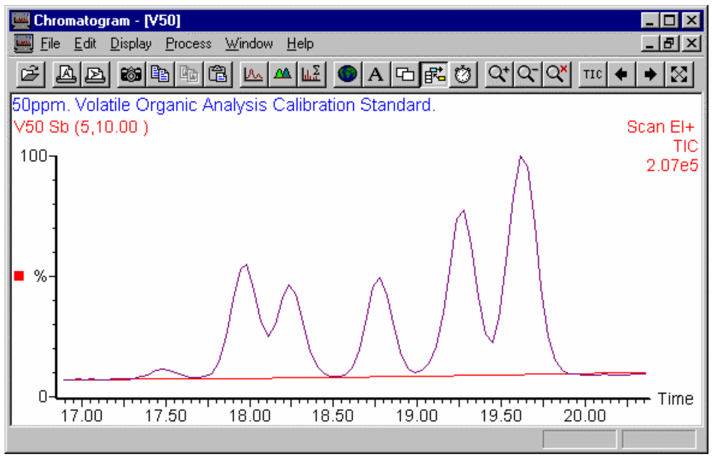
The parameters shown in the figure below produced the background subtracted chromatogram and total ion chromatogram shown in the printed documentation.





You can check the operation of the background subtraction process with a given set of parameters by selecting the **Make graph of fitted polynomial** checkbox. This causes the same calculation to take place, but rather than displaying a chromatogram with the background curve subtracted, the curve itself is displayed. Selecting **Overlay Graphs** and **Link Vertical Axes** from the Chromatogram Display View dialog creates a display similar to that shown.





Subtracting the background from a chromatogram

1. Select **Subtract** from the Chromatogram **Process** menu.
2. Set the polynomial order parameter as described above.
3. Set the below curve parameter as described above.
4. Click **OK**.

The Subtract dialog indicates the progress of the subtract algorithm. After every iteration, TurboMass updates the convergence value in the dialog. The algorithm terminates when convergence is less than tolerance.

With higher order polynomials, background subtract will sometimes have difficulty converging on a solution. There is a preset upper limit of 300 iterations. If background subtract does not seem to be making progress, click **Cancel** in the Background Subtract dialog and try again with a lower-order polynomial.

Smoothing Chromatograms and/or Reducing Noise

Smoothing improves presentation and aids interpretation of a chromatogram by increasing the apparent signal-to-noise ratio.

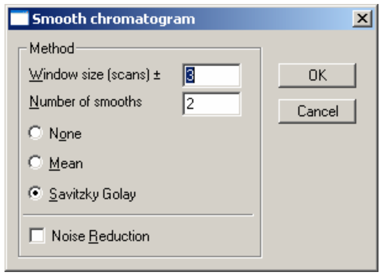
NOTE: *In some instances, if your chromatogram has very small peaks you may want to turn smoothing off to accurately define the valley of overlapping peaks.*

Two types of smoothing are available for chromatograms: Moving **Mean** and **Savitzky Golay**. Both methods slide a window along the chromatogram, averaging the data points in the window to produce a point in the smoothed chromatogram. Moving **Mean** takes the arithmetical mean of the intensities of the data points in the window. **Savitzky Golay** takes an average of the intensities weighted by a quadratic curve. This tends to enhance peak and valley shapes, as well as preserving the height of the peaks better than the Moving **Mean**. However, **Savitzky Golay** does tend to produce small artifacts on either side of the real peaks.

Noise Reduction is optimized for single GC peaks in the signal-to-noise range of 3:1 to 200:1. A window containing multiple GC peaks may lead to a loss of GC peak resolution

Smoothing a chromatogram and/or reducing noise

1. Select **Smooth** from the Chromatogram **Process** menu to open the Smooth chromatogram dialog.



2. Set the **Window size** parameter.

   The number you specify is the half-width of the smoothing window in scans. This parameter can be set automatically by right-clicking and dragging the mouse across a chromatogram peak at half height.

3. Select a Smoothing method (Mean or Savitzky-Golay)

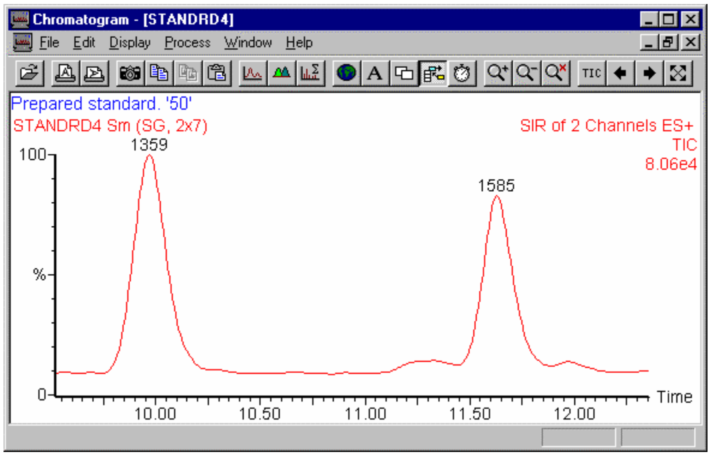
4. As required, adjust the number of times the smooth is repeated by changing the **Number of smooths** parameter.

   Increasing this parameter gives a heavier smooth.

5. Select **Noise Reduction** to apply noise reduction to a chromatogram.

NOTE: *If you only want to apply Noise Reduction without applying smoothing, select None and then select Noise Reduction.*

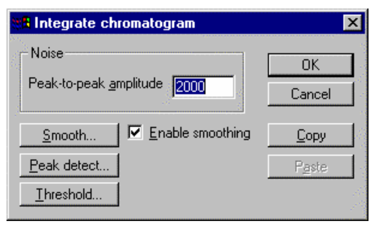
6. Click **OK**.



Integrating Chromatograms

The integration process locates the peaks in a chromatogram, draws baselines, and calculates peak heights and areas for quantification.

You can integrate a chromatogram using the current parameters by clicking . You can use the Integrate chromatogram dialog to change the parameters. The integration process operates only on the currently displayed range and not on the whole chromatogram.



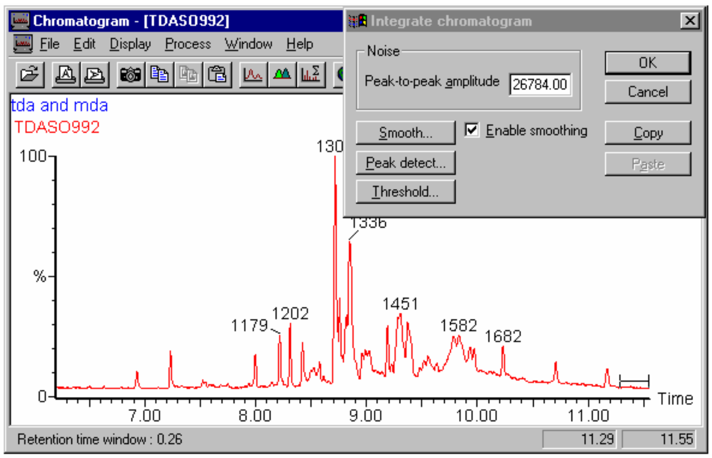
Copy Allows you to copy the current integration parameters to the Clipboard. These parameters can then be pasted into another application such as the Quantify Method Editor.

Paste Allows you to paste a set of integration parameters from the

Clipboard.

Noise Peak-to-peak amplitude

The Integrate chromatogram dialog requires that you enter the **Peak-to-peak Noise amplitude**. This value is used by the integration software to pre-filter the chromatogram. A suitable value can be measured directly from the chromatogram by right-clicking and dragging the mouse across a section of noise in the chromatogram. The sensitivity of the integration algorithm can be fine-tuned by manually adjusting this value. Note that the optimum value is likely to differ for each mass chromatogram.

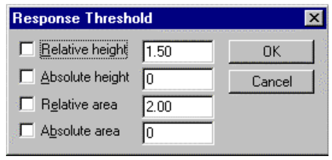


Enable smoothing

You can choose to smooth the chromatogram before integrating by selecting **Enable smoothing**. The parameters for the smooth can be examined and altered by clicking **Smooth**. For more information, see *Smoothing Chromatograms* on page 397.

Threshold

Small peaks can optionally be removed by setting one of the four available threshold parameters. Click **Threshold** to open the Response Threshold dialog, where you can examine or modify these parameters.



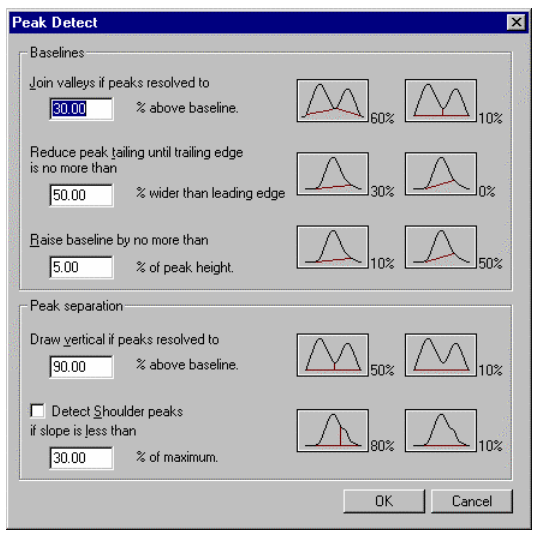
Relative height Removes peaks whose height is less than the specified percentage of the highest peak.

Absolute height Removes peaks whose height is less than the specified value.

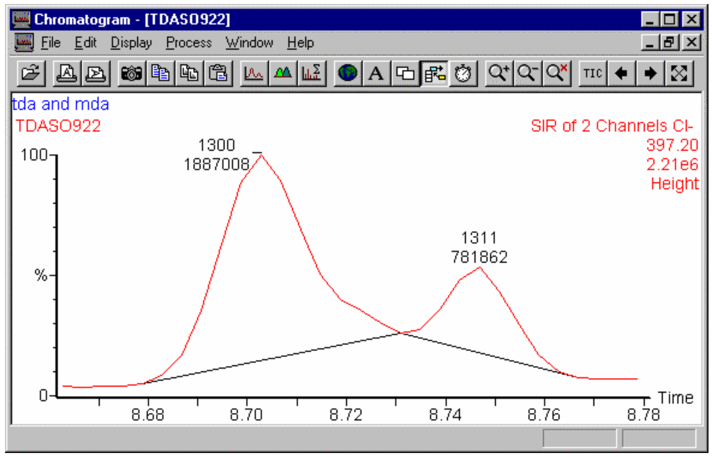
Relative area Removes peaks whose area is less than the specified percentage of the largest peak area.

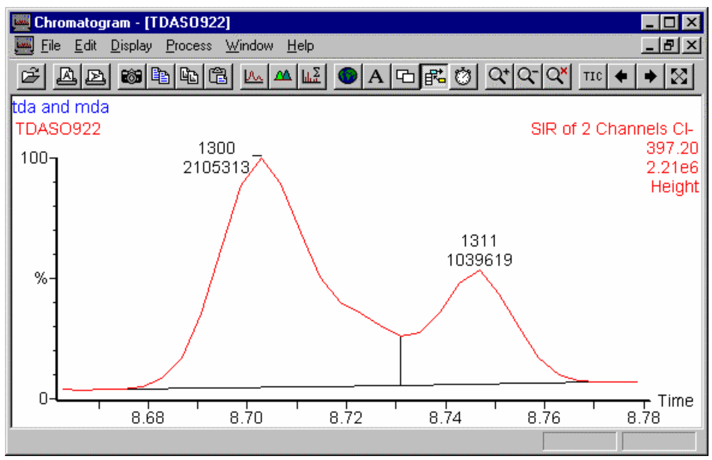
Absolute area Removes peaks whose area is less than the specified value.

You can examine and modify the parameters that control the positioning of baselines and separation of partially resolved peaks by verticals (droplines) by clicking **Peak detect** in the Integrate chromatogram dialog to display the Peak Detect dialog.

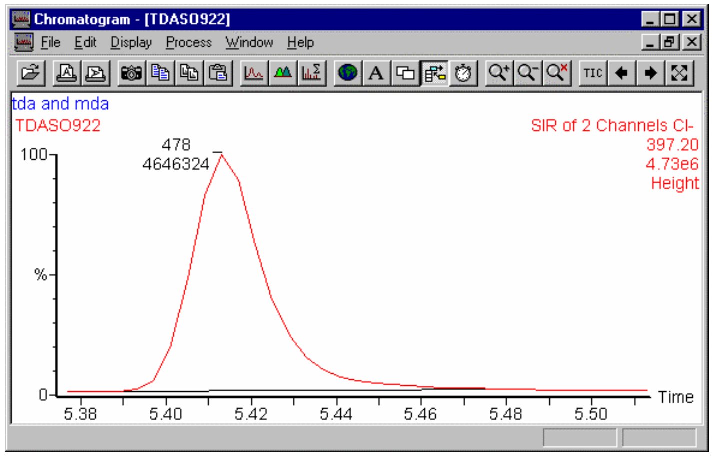


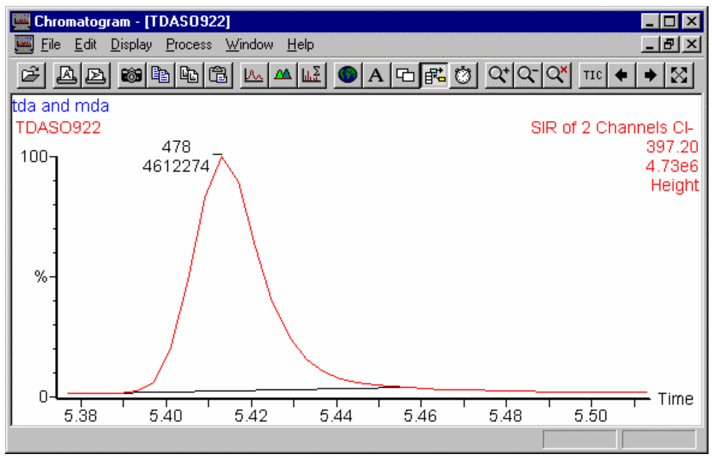
The **Join valleys** parameter affects how baselines for partially resolved peaks are drawn. The larger the value of this parameter, the more peak baselines will be drawn up to the valleys between unresolved peaks. The default value for this parameter is 30 %, and the normal operating range is 5 % - 75 %.



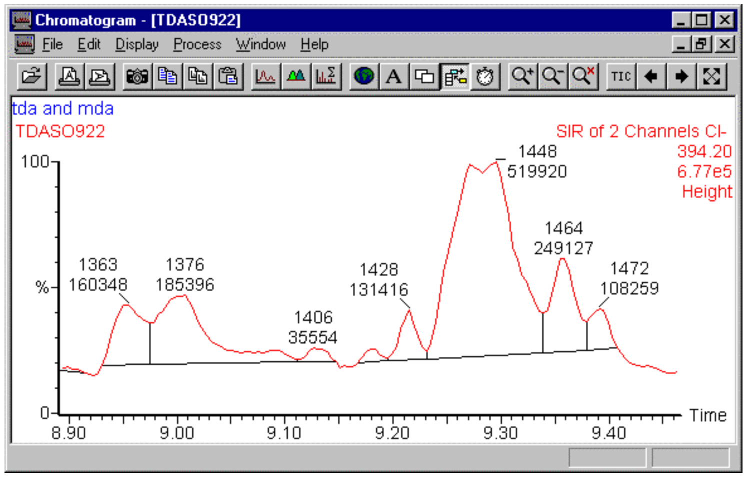


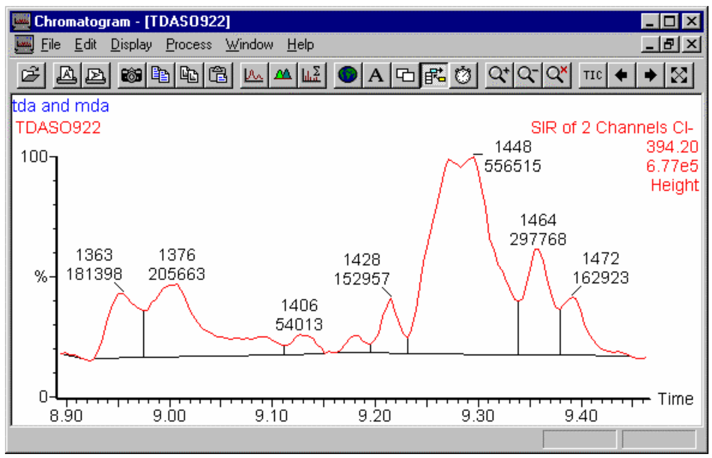
Reduce peak tailing and **Raise baseline** position the baseline end points. In the example, the pronounced tail on the peak at 5.42 min is reduced by decreasing the value of the reduce peak tailing parameter from 150 % to 50 %. The default value for this parameter is 50 %, and the normal operating range is between 25 % and 300 %.



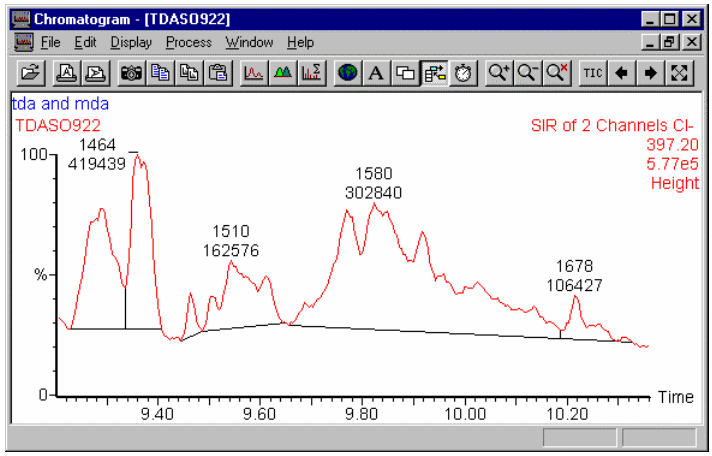


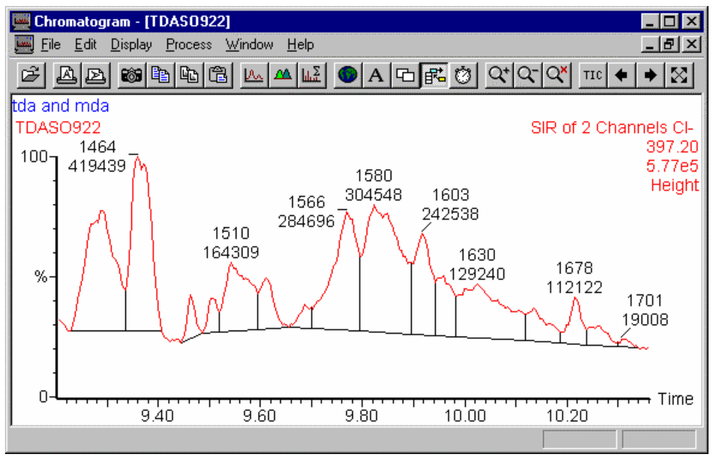
Raise baseline is optionally selected in the Peak Detect dialog, and prevents the baseline end point from being moved too high up the peak. To prevent the baseline endpoints from moving up the peaks, reduce the value of this parameter. The default value is 5 %, and the normal operating range is 5 % - 20 %. This parameter is only relevant when the reduce peak tailing parameter has a small value (less than 50 %). In the example below, the reduce peak tailing parameter has been set to 25 %.





Draw vertical is selected in the Peak Detect dialog, and determines how well resolved peaks must be before they are separated by a dropline (or baselines are drawn up into the valleys, depending on the value of the join valleys parameter). If you want to separate poorly resolved peaks, increase the value of this parameter. The default value is 90 %, and the normal operating range is 50 % - 100 %.





Detect Shoulder peaks is selected in the Peak Detect dialog, and is used optionally to attempt to detect completely unresolved peaks or shoulders. The algorithm will detect a shoulder if the slope of the shoulder top is less than the specified percentage of the steepest slope on the peak. Therefore, to make shoulder detection more sensitive, increase the value of this parameter. The default value is 30 %, and the normal operating range is 20 % - 90 %.

Integrating a chromatogram

1. Display the chromatogram range you want to integrate.

2. Select **Integrate** from the Chromatogram **Process** menu.

3. Enter a value for Noise Peak-to-peak amplitude.

   To calculate this value, display a section of the chromatogram that contains only background. Right-click at one end of a section that contains background noise, and drag the mouse to the other end of the noise section. When the mouse is released, the integration software will calculate the **Noise** amplitude and update the value.

4. Optionally, select **Enable smoothing** and click **Smooth** to examine or modify the smoothing parameters.

5. Optionally, set up one or more thresholds to remove small peaks by clicking **Threshold** in the Integrate chromatogram dialog to open the Response Threshold dialog.

6. Click **OK** to perform the integration.

   The integration software will smooth the chromatogram trace if requested, locate the peaks, draw baselines, and calculate peak statistics.

Editing Detected Peaks

You can use the Edit Integrated Peaks dialog to change the results of integration by changing the position of an individual baseline, adding a single peak, or deleting one or all peaks.

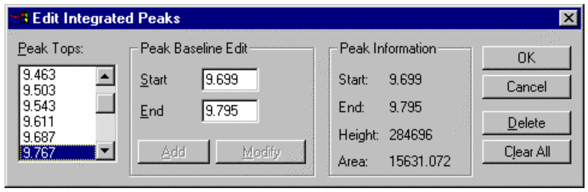
Displaying information about an integrated peak

- Left-click on a peak to display the peak top position, peak height and peak area in the status bar at the bottom of the chromatogram window.

  Peak Annotation can be displayed using any combination of peak top time, peak top scan, peak response height, and peak response area by selecting **Peak Annotation** from the Chromatogram **Display** menu.

Editing a peak baseline

1. Select **Integrated Peaks** from the Chromatogram **Edit** menu to open the Edit Integrated Peaks dialog.



2. Do one of the following to select the peak whose baseline you want to edit:

   - Right-click and select the peak in the Chromatogram display.
   - Select the peak from the **Peak Tops** list in the Edit Integrated Peaks dialog.

3. Modify a baseline range by doing one of the following:

   - Edit the **Start** or **End** values.
   - Right-click and select a range, and click **Modify**.
   - Left-click on one of the end markers (boxes) and drag it to the required position.

4. The values in **Peak Information** will be updated to reflect the edited baseline.

Adding a new peak

1. Select **Integrated Peaks** from the Chromatogram **Edit** menu to open the Edit Integrated Peaks dialog.
2. Enter the **Start** and **End** points of the baseline for the new peak, or right-click and select a range.
3. Click **Add** to update the values in **Peak Information** to reflect the new peak.

Deleting a single peak

1. Select **Integrated Peaks** from the Chromatogram **Edit** menu to open the Edit Integrated Peaks dialog.

2. Do one of the following to select the peak you want to delete:

   - Right-click and select the peak in the Chromatogram display.

   - Select the peak from the **Peak Tops** list in the Edit Integrated Peaks dialog.

3. Click **Delete**.

Deleting all the peaks

1. Select **Integrated Peaks** from the Chromatogram **Edit** menu.

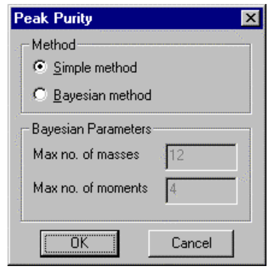
2. Click **Clear All** in the Edit Integrated Peaks dialog.

3. When you are satisfied with your changes, click **OK**.
   Clicking **Cancel** aborts the edit and discards your changes.

Peak Purity

The Peak Purity process works on TIC chromatograms that have already been integrated. Note that it is important not to have **Enable Smoothing** selected in the Integrate chromatogram dialog; this is because smoothing tends to increase the peak width, and hence when the Purity process selects scans from the edges of the smoothed peak, the scans that are chosen are actually in the noise portion of the raw data. Since it is the raw data that is used for the purity calculation, this will have the effect of artificially depressing the purity value for each peak.

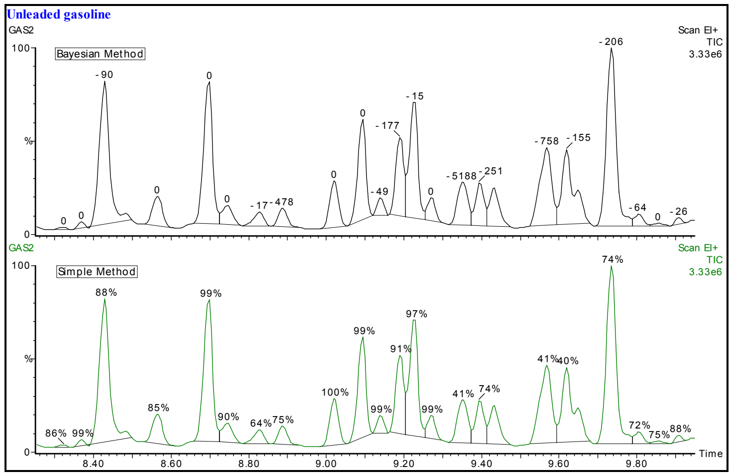
Select **Peak Purity** from the Chromatogram **Process** menu to open the Peak Purity dialog.



There are two separate methods for calculating Peak Purity.

The first, called the **Simple method**, requires no parameters. It selects five spectra from across the peak and correlates each spectrum with the other spectra. The mean correlation value is displayed, scaled to a percentage (0 % - 100 %), with 100 % representing total purity, and 0 % total impurity. A purity value of 60 % does not mean that the peak has two components in the ratio 60 : 40.

The second method, called the **Bayesian method**, requires two parameters. This method characterizes each mass channel as a set of (up to) its first four moments. The first moment represents peak position, the second peak width, and the third asymmetry. The program can be restricted to use less than four moments by reducing the **Max no. of moments** parameter. Reducing this value will decrease the run time of the process. It is also possible to reduce the number of mass peaks used for comparison. This value is represented by the **Max no. of masses** parameter. Decreasing this parameter will also result in reduced run time. The Bayesian method is based on a rigorous probabilistic analysis. The output value loosely represents the natural logarithm of the probability that the peak is pure. Therefore, to calculate the probability that a peak with purity value x is pure, evaluate exp(x). This implies that the maximum score (100 % probability pure) is 0.



Calculating the peak purity index for a Total Ion Chromatogram

1. Display the chromatogram range of interest in a chromatogram window.

2. Integrate the chromatogram, remembering to disable smoothing.

3. Select **Purity** from the Chromatogram **Process** menu to open the Peak Purity dialog.

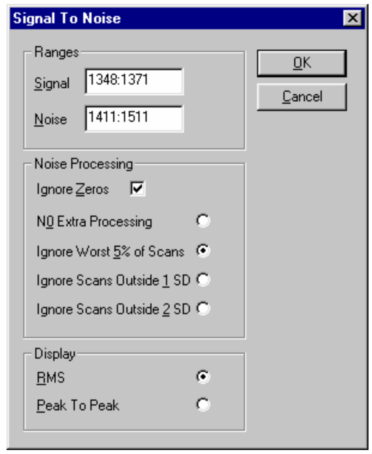
4. Select the purity method, either **Simple** or **Bayesian**.

   For the Bayesian method, optionally enter the number of moments to use and the number of mass spectral peaks to consider.

5. Click **OK**.

Signal to Noise

It is sometimes useful to know the ratio of the peak heights to the level of noise in a mass chromatogram. TurboMass provides the Signal to Noise calculation to do this. Signal to Noise can be accessed from Chromatogram by selecting **Signal to Noise** from the **Process** menu.



The Signal to Noise (S/N) calculations can be carried out to display peak to peak or RMS (root mean square) values. If Peak-to-Peak is required, the greatest height of the signal range above the mean noise value is divided by the variance. If RMS is required, the greatest height of the signal above the mean noise is divided by the root mean square deviation from the mean of the noise. The S/N calculated using RMS noise is usually expected to be about 5 times the S/N value calculated using Peak-to-Peak noise.

Various authorities have different methods for determining what level of noise is taken into account for the calculations of noise variance and RMS deviation. A two-step process is carried out. First, the mean should be calculated with or without zeros as normal. Optional processing then allows three options:

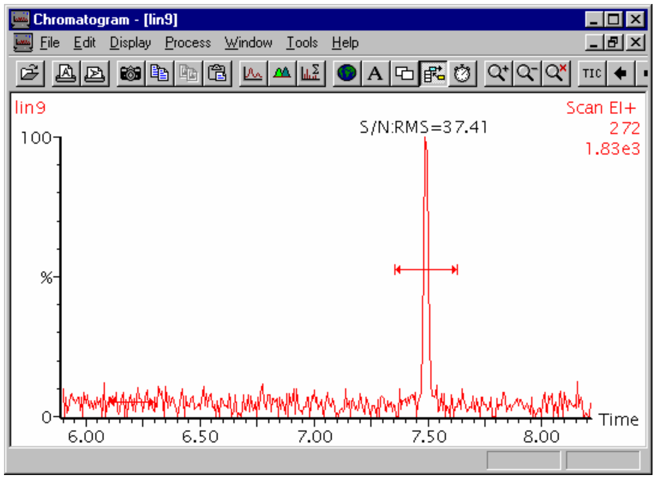
Ignore Worst 5 % of Scans The 5 % of scans that have the greatest deviation from the mean are disregarded in the noise signal.

Ignore Scans Outside 1 SD Those scans whose deviation from the mean is greater than one standard deviation are disregarded in the noise signal.

Ignore Scans Outside 2 SD Those scans whose deviation from the mean is greater than two standard deviations are disregarded in the noise signal.

Options 1 and 3 are expected to give roughly equivalent results. Option 2 should give an RMS value of about double that of the other two options.

If one of these three processing options is selected, then the mean and RMS deviation of the noise are recalculated disregarding the appropriate points.



Calculating the signal to noise value for a Mass Chromatogram

1. Display the chromatogram range of interest in a chromatogram window.

2. Select **Signal to Noise** from the Chromatogram **Process** menu.

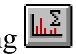
3. Enter **Signal** and **Noise** ranges.

   Either enter values or, right-click at one end of the Chromatogram region of interest, and drag the mouse horizontally to the other end. TurboMass indicates the range you have selected. The dialog will be updated to show this range.

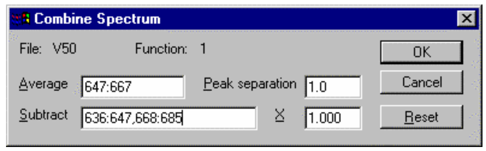
4. Select the **Noise Processing** and **Display** methods required.

5. Click **OK**.

Combine Spectra

The Combine process (also called spectral background subtraction) can be accessed from either Chromatogram or Spectrum by clicking  or by selecting **Combine** from the **Process** menu.

The combine process operates on centroid-mode or continuum data. Its purpose is to produce a single scan from all the scans across a TIC peak. The combined scan exhibits enhanced signal-to-noise and improved mass accuracy.

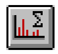


Specify three scan ranges and a background factor. One range contains the scans across the peak top and the other two ranges contain scans from the background, on each side of the peak. The scans across the peak top are averaged together and the average of all the background scans, multiplied by the background factor (X), is subtracted from the result.

The **Peak separation** parameter is the spectral peak width in Da (amu). For centroided data, the peak width can be determined from inspection of the tune peaks on the Tune page. It is typically 1.0 for GC/MS data. The Combine algorithm combines peaks within a Peak separation window into a single peak. Clicking **Reset** will remove all values that have been entered into the dialog.

Combining scans in a centroid-mode data file

1. Display the chromatogram peak of interest in a chromatogram window.

2. Click 

   OR

   Select **Combine Spectra** from the Chromatogram **Process** menu to open the Combine Spectrum dialog.

3. Enter the peak top scan range either by entering scan numbers separated by a colon (for example, 619:626) into the **Average** field, or by right-clicking and dragging the mouse across the peak.

4. Optionally, enter one or two background scan ranges:

   Enter the scan numbers into the **Subtract** field. Each range should be in the form of two numbers separated by a colon, as above; and if there are two ranges, they should be separated by a comma (for example, 606:612,631:637).

   OR

   Right-click and drag the mouse across the first background scan range. Optionally repeat for a second range.

5. Optionally, enter a background factor in the **X** field.

6. Optionally, enter a **Peak separation** value.

7. Click **OK**.

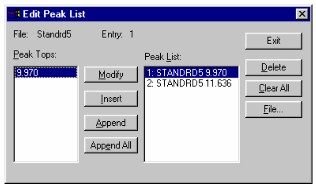
Peak Lists

The results of the peak integration can be saved to disk as a named Peak List. Peak Lists can then be processed using the TurboMass Quantify program.

Creating and Editing a Peak List

Use the following procedures to create a new peak list or edit an existing one.

1. Select **Peak List Write** from the Chromatogram **Edit** menu to display the Edit Peak List dialog.



2. Click **File** to display the File Open dialog, and select a file.

3. If you want to create a new **Peak List** file, enter a new name into the File Name field, and click **Open**.

4. Click **Exit**.

Appending a single peak to the current Peak List

1. Select **Peak List Write** from the Chromatogram **Edit** menu to display the Edit Peak List dialog.

2. Select the peak you want to append either from the **Peak Tops** list, or by right-clicking the peak in a chromatogram trace.

3. Click **Append**.

   The contents of the **Peak List** list will be updated to include the new peak.

4. To append all the peaks in the **Peak Tops** list, click **Append All**.

Deleting a single peak from the current Peak List

1. Select **Peak List Write** from the Chromatogram **Edit** menu to display the Edit Peak List dialog.
2. Select the peak you want to remove from the **Peak List** list.
3. Click **Delete**.
4. To delete all the peaks in the peak list, click **Clear All**.

Reading a Peak List into a Chromatogram

Use the following procedures to select a peak list file and read a single peak or the entire peak list into the currently selected chromatogram.

Selecting a Peak List file

1. Select **Peak List Read** from the Chromatogram **Edit** menu.
2. Click **File** to display the File Open dialog.
3. Select a file from the list and click **Open**.
4. Click **OK**.

Reading a single peak into the currently selected chromatogram

1. Select **Peak List Read** from the Chromatogram **Edit** menu.
2. Select a peak from the **Peak List** list.
3. Click **OK**.

Reading a whole peak list into the currently selected chromatogram

1. Select **Peak List Read** from the Chromatogram **Edit** menu.
2. Click Get All.
3. Click **OK**.

Automatic Library Searching

This option automatically searches the specified library for entries that match the currently integrated chromatogram displayed in the Chromatogram window. This process uses your current integration and library search parameters.

Note that while automatic library searching can work well for chromatographically well-resolved peaks, complex chromatograms will probably require manual background subtraction and library searching.

Performing an automatic library search

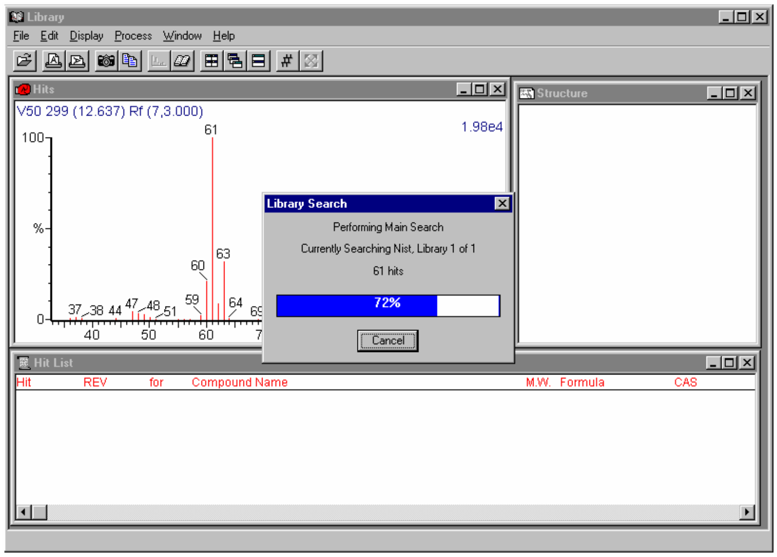
1. In the Chromatogram window, set the display range and integration threshold values to limit the integrated peaks to only those you wish to library search.

   See Integrating Chromatograms on page 399 to set up your integration parameters.

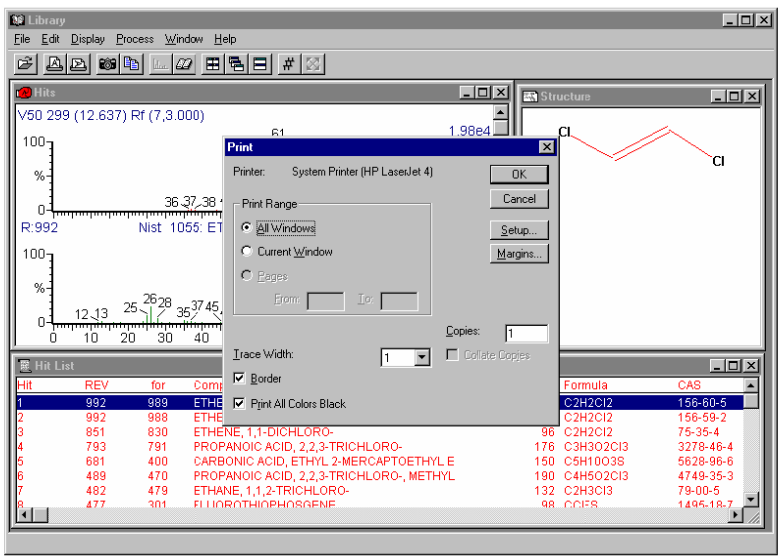
2. Set up your Library search and display parameters.

   For more information, see the fully- and semi-automatic library search procedures in *Library* on page 485.

3. Click  to initiate the automatic library search process for the first peak in the integrated chromatogram.



As the search process progresses, TurboMass displays a Print dialog where you can specify whether you want to print out the current window or all windows for that peak.



TurboMass continues to search the specified library for consecutive peaks in the integrated chromatogram and prints the results of each search.

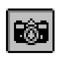
Copying to and from the Windows Clipboard

The Windows Clipboard provides temporary storage for information that is being transferred between application programs (word processors, spreadsheets, TurboMass etc.). You can use the Clipboard to move data into or out of the Chromatogram window, either as a picture or as a text list. For example, you can paste spectra or chromatograms into reports written with a Windows compatible word processor.

TurboMass now copies a Chromatogram picture to the Clipboard as a metafile giving greatly improved resolution. When the metafile is pasted into another Windows application it can be rescaled if required without distorting the original image as long as the original aspect ratio is maintained. When you use the TurboMass Edit Copy Picture command both a metafile and a bitmap are copied to the Windows Clipboard.

Copying a chromatogram as a picture to the Clipboard

1. Produce the required display in a chromatogram window.

2. Click 

   OR

   Select **Copy Picture** from the Chromatogram **Edit** menu to copy the contents of the window to the Clipboard as both a metafile and a bitmap.

3. To read the image into another application as a metafile, select **Paste** from the other application's **Edit** menu. If you select **Paste Special** from the other application's **Edit** menu, you will be given the option of pasting either the metafile or the bitmap.

Copying a chromatogram as a text list to the Clipboard

1. Display the required time range in a chromatogram window.

2. Click 

   OR

   Select **Copy Chromatogram List** from the Chromatogram **Edit** menu. The section of the chromatogram on display will be transferred to the Clipboard as (time, intensity) pairs or (scan, intensity) pairs depending on the horizontal axis setting.

3. To read the information into another application, select **Paste** from the other application's **Edit** menu.

Copying integrated chromatogram peaks as a text list to the Clipboard

1. Display the required time range in a chromatogram window

2. Click  or select **Copy Detected Peaks** from the Chromatogram **Edit** menu. The chromatogram peaks on display will be transferred to the Clipboard. The information transferred for each peak is the peak top, height, area, start, end, start height, and end height.

3. To read the information into another application, select **Paste** from the other application's **Edit** menu.

Pasting information into a chromatogram window from the Windows Clipboard

1. Click 

   OR

   Select **Paste** from the Chromatogram **Edit** menu to paste the default Clipboard object to chromatogram. Select **Paste Special** to choose which object to paste into Chromatogram. These objects would typically be metafiles, bitmaps, or text.

2. Drag the outline of the image to the required position with the mouse.

   You can paste the contents of the Clipboard, whether a bitmap, a metafile, or text, into a chromatogram window. If the data are in textual or metafile form, you can re-scale it using the mouse and there will be no distortion of the image. However, if you paste a bitmap, re-scaling is done by stretching the image, which will cause some distortion. To avoid this, scale the image to the required size before you copy it to the Clipboard.

Removing pasted input from the display

1. Select the item you want to remove.

2. Press the DELETE key.

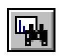
Spectrum 14

Getting Started

You can open the Spectrum window in several ways.

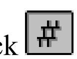
Displaying the first scan of the current data file

To display the first scan of the current data file, do one of the following:

- Double-click at the required retention time in the Chromatogram window.
- Right-click and drag the mouse across the appropriate range of interest in the Chromatogram window to initiate a Combine Spectrum process.
- Select **Spectrum** from the TurboMass **View** menu.
- Click .
- Enter CTRL+S.

Displaying a particular scan in the current file

To display a particular scan in the current file, do one of the following:

- Use the mouse to select the required part of a scan in a chromatogram.
- Click  from the Spectrum toolbar and enter the required scan number.
- Select **Spectrum…At** from the Spectrum **Display** menu and enter the required scan number.

About the Display

The spectrum application runs in a top level window that has a menu bar at the top. Under each of the headings on the menu bar is a drop-down menu, and you can

access every feature of the Spectrum application from this menu structure. The commands and icons are quite similar to those in Chromatogram.

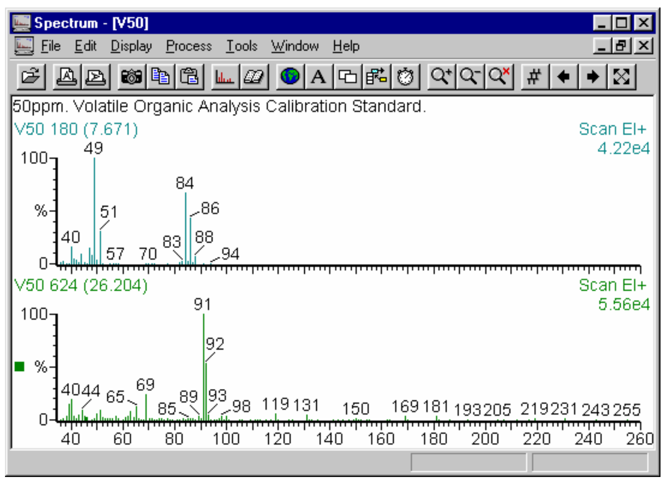
At the top of the spectrum window is the toolbar. The toolbar provides a quick way of performing common operations.

The top level window can contain one or more spectrum windows, and each can contain one or more spectrum traces.

The current spectrum window is identified by a colored title bar. To select another window to be the current one, either click in any part of the new window, or select one from the bottom section of the **Window** menu.

When there is more than one trace in a window, the current one is identified by a colored square on the left of the trace. To select another trace to be the current one, left-click any part of the trace, select one from the Graphs option on the Spectrum **Display** menu, or use the up and down arrow keys on the keyboard.

The spectra in each spectrum window share a common mass axis. To display spectra on different mass axes, you must put them in separate windows.



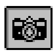
The Spectrum Toolbar

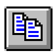
The toolbar displayed at the top of the spectrum window lets you perform some common operations with a single click of the appropriate toolbar button. The default Spectrum toolbar contains the buttons listed below. You can also customize the Spectrum toolbar and add additional buttons for other Spectrum operations.

 Opens a data file.

 Prints the current window in portrait format.

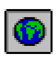
 Prints the current window in landscape format.

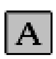
 Sends a picture of current window to the Clipboard.

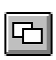
 Copies a list of points in the spectrum to the Clipboard.

 Pastes the contents of the Clipboard onto the display.

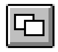
 Identifies the current scan using the library search facility.

 Toggles between processing all traces in the current window and the current trace in the current window.

 Writes text onto a spectrum. After clicking this button, point to where text is required, and left-click. The Edit Text String dialog appears for text input. When **OK** is clicked, the text is written to the Spectrum display.

 Selecting once causes each subsequent spectrum to appear in a new spectrum window, rather than being added to the current window. Selecting a second time cancels this mode.

 Selecting once causes each subsequent spectrum or spectrum process to replace the currently selected trace. Selecting a second time causes each subsequent spectrum or spectrum process to be added to the traces on display.

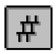
NOTE:  *is unavailable when*  *is clicked.*

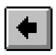
 Toggles real time spectrum update on and off.

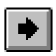
 Increases magnification of current range.

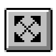
 Decreases magnification of current range.

 Deletes current magnification range.

 Selects a new scan from the current data file.

 Decrements the currently displayed scan.

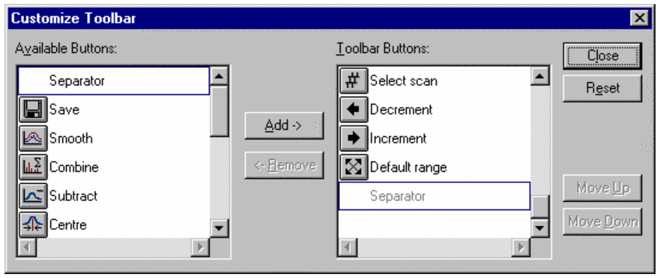
 Increments the currently displayed scan.

 Click once to restore the previous display range; click again to use the default display range.

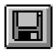
Customizing the Spectrum Toolbar

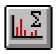
The Spectrum toolbar can be customized to add other buttons for the operations that you use most frequently, remove buttons you do not require, and determine the order in which the toolbar buttons are displayed. In this way you can customize the TurboMass display to suit the way you work.

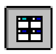
To customize the Spectrum toolbar, select **Customize toolbar** from the Spectrum **Display** menu.



The additional buttons that can be added to the default Spectrum toolbar are:

 Save spectrum.

 Combine spectra.

 Tile windows.

 Cascade windows.

 Stack windows.

Adding buttons to the toolbar

1. Select the button you want to add to **Available Buttons** list.

2. In the **Toolbar Buttons** list, select the toolbar button before which you want to insert the new button.

3. Click **Add** to add the new toolbar button.

   Repeat Steps 1 - 3 as often as required.

4. Separators can be inserted between toolbar buttons to divide them into logical groups. To add a separator repeat steps 1 - 3 and then select **Separator** in **Available Buttons**.

5. Click **Close** to exit and save changes.

Removing buttons from the toolbar

1. In the **Toolbar Buttons** list, select the button you want to remove.
2. Click **Remove** to remove the button.
   Steps 1 and 2 can be repeated as often as required.
3. Click **Close** to exit and save changes.

Changing the order in which toolbar buttons are displayed

1. In the **Toolbar Buttons** list, select the button you want to move.
2. Click **Move Up** or **Move Down** to move the toolbar button.
   Steps 1 and 2 can be repeated as often as required.
3. Click **Close** to exit and save changes.

Resetting the toolbar to default settings

1. Click **Reset**.
2. Click **Close** to exit and save changes.

Removing the toolbar from the Spectrum display

Select **Toolbar** from the Spectrum **Display** menu to display/hide the toolbar. This command is a toggle.

A check mark will appear next to this menu item when it has been selected.

Displaying Spectra

The following procedures describe how to display spectra in the same or separate windows.

Adding or Replacing Spectra

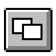
TurboMass gives you a number of options for displaying any new spectrum traces. New spectrum traces can be generated by:

- Opening a new file.
- Processing spectra (subtract, smooth, center etc.).
- Selecting spectra by double-clicking on a chromatogram.

Once generated, you can display spectra in the same or in separate windows.

When new traces are displayed in the same window, you can choose whether to add the new trace to the traces currently displayed or to replace the current trace with the new trace.

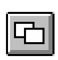
Displaying spectra in a new or in the same window

Toggle  to display each new spectrum trace in a new or in the same window.

Adding or replacing spectra in a window

Toggle  to replace or add each subsequent spectrum or spectrum process in the current window.

Up to 16 spectrum traces can be displayed in one window.

NOTE:  *is unavailable when*  *is clicked.*

Manipulating the Display

The following procedures describe how to alter the mass and intensity axes.

Changing the range of the mass axis

To change the range of the mass axis, do one of the following:

- Left-click at one end of the region of interest, and drag the mouse horizontally to the other end. TurboMass will indicate the range you have selected; do not go beyond the bounds of the axis. When the mouse is released, the selected range will be redisplayed to fill the current window.

- To expand the spectral range of interest, left-click and click  as many times as required to achieve the desired magnification. Click  to restore the original range. Repeat this operation as often as required.

- Change the range of the mass axis from the menu:

    1. Select **Range From** from the Spectrum **Display** menu.

    2. Enter new **From** and **To** values for the mass axis.

    3. Click **OK**.

Changing the range of the intensity axis

Left-click at one end of the region of interest, and drag the mouse vertically to the other end. TurboMass will indicate the range you have selected; do not go beyond the bounds of the axis. When the mouse is released, the selected range will be redisplayed to fill the current window.

This operation can be repeated as often as required.

Setting Magnified Ranges

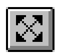
You can set magnification ranges in several ways.

Creating magnification ranges using mouse and menu commands

- If you have a three-button mouse, middle-click at one end of the region of interest and drag the mouse horizontally to the other end. As you drag the mouse, TurboMass will indicate the range you have selected. When the mouse is released the selected range will be redisplayed with an initial magnification factor of 2.

- Hold down the SHIFT key, and left-click and drag across the region of interest.

- To expand the spectral range of interest, left-click and drag the mouse, and click  as many times as required to achieve the desired magnification.

  Click  to restore the original spectral range.

- Create single or multiple magnification ranges using the **Magnify** menu command:

  1. Select **Magnify** from the Spectrum **Display Range** menu, or double-click the magnify range indicators of an existing magnified range to open the Spectrum Magnify dialog.

  2. Enter the range you want to magnify in **From** and **To**. Enter the magnification factor you want to apply in **By**.

  3. To define more than one magnification range, select a new range in the **Range** field and repeat step 2.
  4. You can define up to five different magnified regions of the spectrum.

  5. Click **OK** to exit.
  6. The spectrum is redisplayed with the data in the selected regions magnified by the requested factor. The magnified regions are displayed in a different color and labeled with the magnification factor.

Magnifying the range of the intensity axis using the toolbar

Use one of the following tool buttons to magnify the intensity axis range.

 Increases magnification of the current range. The current magnification factor is multiplied by 1.5 and rounded up to the nearest even number to give the increased magnification factor. If the initial magnification factor is 2, this will give subsequent magnification factors of 4, 6, 10, 16, etc.

 Decreases magnification of the current range. The current magnification factor is divided by 1.5 and rounded down to the nearest even number to give the decreased magnification factor. If the initial magnification factor is 16, this will give subsequent magnification factors of 10, 6, 4, etc.

 Deletes the current magnification range.

Where multiple magnification regions have been defined, to select the current magnification range click in the magnification description that appears above the range. The description will change color to red to indicate the currently selected range.

Changing the magnification of a particular range

Double click on the magnification description of the magnification range. The Spectrum Magnify dialog will be displayed. Enter the new magnification factor and click **OK** to exit.

Deleting Magnification Ranges

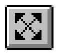
- To delete a single magnification range, select the range you want to cancel and click .
- To delete all magnification ranges, select **Magnify** from the Spectrum **Display Range** menu. Click **Default** to delete all magnification ranges. Click **OK** to exit.

Changing the Range of Both Axes

➢ Left-click at one corner of the region of interest, and drag the mouse vertically to the diagonally opposite corner. As you drag the mouse TurboMass will indicate the region you have selected; do not go beyond the bounds of the axis. When the mouse is released, the selected region will be redisplayed to fill the current window.

This operation can be repeated as often as required.

Restoring the Display

➢ Toggle  to restore the display to its previous state or to the default range.

OR

Toggle the Default command in the Spectrum **Display Range** menu to restore the display to its previous state or to the default range.

These operations do not remove magnification ranges.

Setting the Display Range Defaults

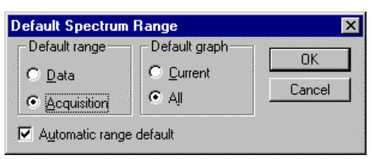
The display range default settings specify both the effect of clicking  and adding a new spectrum to the display.

Changing the default display

1. Select **Range, Default** from the Spectrum **Display** menu.

2. Make any changes.

3. Click **OK**.



Default range Only relevant to Centroid mode acquisitions. Specifies whether the mass axis will range from the first peak in the scan to the last peak in the scan (Data), or over the range you requested when the acquisition started (Acquisition).

Default graph If there is more than one spectrum in the same window, this option specifies whether the default mass range for that window is made large enough to include the mass ranges of all the spectra, or the current spectrum only.

Automatic range default If enabled, the display range will return to the specified default (see **Default range** and **Default graph**) when a new spectrum is added to a spectrum window. If **Automatic range default** is disabled, the display range will remain unchanged when a new spectrum is added.

Displaying a Spectrum as a List

You can replace the display in the current spectrum window with a list of masses and intensities of the peaks in the currently selected spectrum.

Select **List Spectrum** from the Spectrum **Display** menu.

A check mark is placed next to the **List Spectrum** menu item. You can use most of the menu commands and the spectrum toolbar.

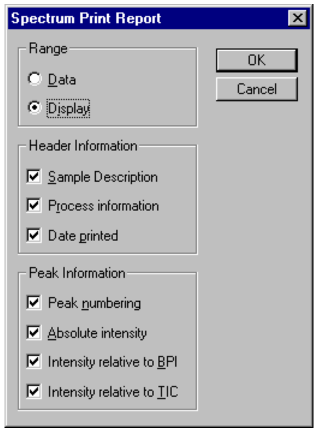
Restoring the graphical display

Select **List Spectrum** from the Spectrum **Display** menu.

The check mark is removed from the **List Spectrum** menu item.

Printing a report of the spectrum listing

1. Select **Print Report** from the Spectrum **File** menu.



2. Select the data range you want to display.

   Select **Data** to print a listing of the whole data file. Select **Display** to print a listing of the current display range.

3. Select the relevant **Header Information** and **Peak Information** options you want to print.

4. Click **OK** to exit and print the report.

Printing with Chromatogram

This prints the active spectrum and chromatogram on the same page to the default printer. To Print the Active Spectrum and Chromatogram on the same page:

1. Open the raw file and selected function in the Chromatogram window.

2. Scale the chromatogram as desired.

3. Set up peak annotations as desired.

4. Select the scan desired or perform a Combine operation (background subtraction).

5. Set up annotations in the Spectrum window as desired.

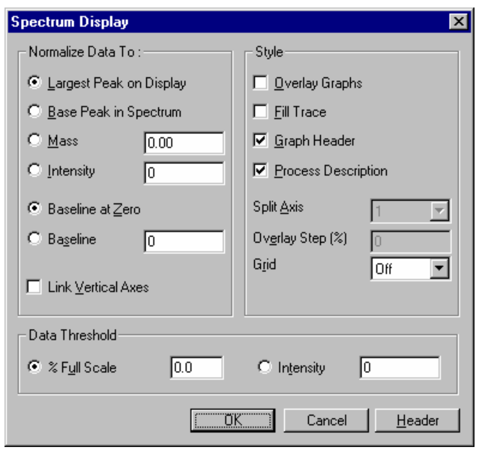
6. Choose the **Print With Chromatogram** command from the File menu in the Spectrum window.

Controlling the Appearance of the Display

Each spectrum window has its own set of Display Parameters, which determine the appearance of the spectrum display. You can inspect and alter the parameters for the current spectrum window from the Spectrum Display dialog.

Changing the display parameters

1. To display the Spectrum Display dialog, select **View** from the Spectrum **Display** menu.



2. Make any changes to the following parameters and click **OK**.

Normalize Data To

This set of parameters specifies the scale on the intensity axis.

Largest Peak If selected, then 100 % on the intensity axis represents

on Display — the intensity of the most intense peak currently on the display.

Base Peak in Spectrum — If selected, then 100 % on the intensity axis represents the intensity of the most intense peak in the spectrum.

Mass — If selected, then 100 % on the intensity axis represents the height of the peak at the specified mass.

Intensity — If selected, then 100 % on the intensity axis represents the specified intensity.

Baseline at Zero — If selected, the vertical axis is scaled from 0 %

Baseline — If you select **Baseline** and specify an intensity offset, the vertical axis is scaled from your specified intensity. This option can be useful for displaying spectra that have a raised baseline.

Link Vertical Axes — When comparing two spectra by overlaying them on the same mass scale, it may be useful to plot both spectra on the same intensity scale also. **Link Vertical Axes** allows you to do this; if you select this option all axes in the current window will be given a common vertical scale.

Data Threshold

When processing centroid type data, it can be useful to specify an intensity threshold. Peaks whose intensity is less than the threshold will not be displayed. There are two methods of specifying a threshold:

% Full Scale — Allows you to set a threshold as a percentage of the intensity of the largest peak in the spectrum.

Intensity — Allows you to set an absolute intensity threshold.

The threshold parameters are not applicable to continuum mode data.

Style

Overlay Graphs If selected, multiple traces in the same window will be superimposed on the same axis. If deselected, the traces will be drawn on separate axes, arranged vertically. When spectra are overlaid only the currently selected trace is annotated.

Fill Trace If selected, the area under the spectrum trace will be colored. This option only applies to continuum-type (not centroid) data.

Graph Header Allows you to turn off the header information normally displayed at the top of the spectrum in order to produce data for publication. If selected, the header will be displayed; if deselected, the header will not be displayed.

Process Description Each process performed on a spectrum adds a summary of its parameters to the spectrum's header. The **Process Description** option allows you to turn off only the process information, and leave the remainder of the header on the spectrum.

Graph Header over-rides **Process Description**. That is, if the **Graph Header** is turned off, the **Process Description** will be as well.

Split Axis Is enabled when **Overlay Graphs** is selected. **Split Axis** allows you to change the aspect ratio of the spectrum by dividing the mass axis into segments, then arranging the segments vertically. For example, if a spectrum from 40 to 340 amu is on display, and you select 3 from **Split Axis**, the display will show three axes, one from 40 to 140 amu, one from 140 to 240 amu, and one from 240 to 340 amu.

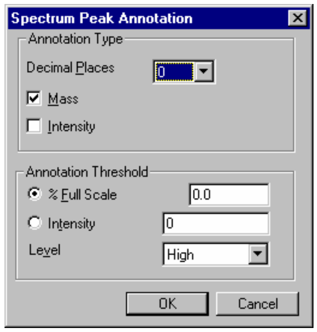
Overlay Step (%)	The **Overlay Step X (%)** and **Overlay Step Y (%)** parameters are enabled when **Overlay Graphs** is selected. **Overlay Step (%)** allows you to offset each subsequent spectrum trace by a percentage of the corresponding axis, which can make it easier to examine overlaid traces. Entering a value in the **X** field will offset each new trace horizontally. Entering a value in the **Y** field will offset each new trace vertically. Entering values in both will offset each new trace diagonally.
Grid	Allows you to fit a grid to the Spectrum display. The pattern of the lines that make up the grid can be chosen as Dot, Dash, or Solid.
Header	Clicking **Header** displays the Header Editor, which allows you to edit the header information displayed at the top of the window.

Controlling the Appearance of Peak Labels

Each spectrum window has its own set of Peak Annotation parameters that determine the appearance of peak labels. You can inspect and change the parameters for the current spectrum window from the Spectrum Peak Annotation dialog.

Changing the peak annotation parameters

1. Select Peak Annotation from the Spectrum **Display** menu.
2. Make any changes.
3. Click **OK**.



Annotation Type

Decimal Places Affects the precision to which mass labels are displayed. You can select between zero and four decimal places on masses. This parameter does not affect intensity labels, which are always displayed as integers. In general, only one decimal place is significant for quadrupole GC/MS data, and usually none are displayed.

There are several types of peak labels. Some are always available; others are the result of a specific process. All can be controlled separately by means of a set of checkboxes.

Mass If selected, peaks in the current spectrum window will be labeled with their masses to the specified number of decimal places.

Intensity If selected, peaks in the current spectrum window will be labeled with their intensity as an integer value.

Annotation Threshold checkboxes allow you to specify a minimum intensity for a peak to be labeled.

% Full Scale Allows you to set a threshold as a percentage of the base peak intensity.

Intensity Allows you to set an absolute intensity threshold.

Level Determines the number of labels that appear on the chromatogram. The level can be set to High, Medium, or Low.

Annotating a particular peak

- Hold down the CTRL key and right-click the peak you want to annotate with the mass label.

- To remove the mass label from the peak, hold down the CTRL key and right-click the peak a second time.

Removing Spectra from the Display

You can remove the currently selected spectrum by pressing the DELETE key. A dialog will ask you to confirm the deletion. Clicking **OK** will remove the spectrum from the display. This operation does not affect the data stored on disk.

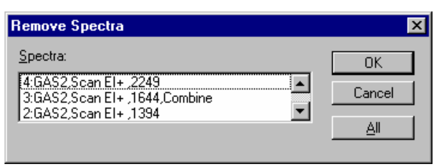
You can also remove traces using the Remove Spectra dialog. This is a faster method if you want to remove more than one spectrum.

Removing multiple spectra from the display

1. Select **Remove** from the Spectrum **Display** menu.

2. The spectra in the current window are listed in the order in which they appear on the display. You can select one or more spectrum by clicking in the list. Clicking again on a selected item will cancel the selection. You can select all the spectra by clicking **All**.

3. Click **OK** to exit.



Real-time Display of Spectra

You can display each new spectrum as a data file is being acquired by clicking  or by selecting **Real-Time Update** from the Spectrum **Display** menu.

Each spectrum window has a separate real time update switch. You can see the state of the switch for a particular window by seeing if  is selected or by making that window current, then choosing the Spectrum **Display** menu. If real-time update is enabled for the current window, **Real-Time Update** has a check mark next to it.

Changing the Order of Displayed Spectra

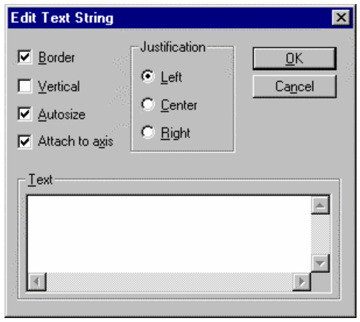
When a window contains multiple traces, you can change the order in which spectra are displayed. The first spectrum in the list is displayed at the bottom of the window. The first spectrum is displayed on top of the others, if traces are overlaid.

Select **Move To First** from the Spectrum **Display** menu to display the currently selected spectrum at the bottom of the display.

Select **Move To Last** from the Spectrum **Display** menu to display the currently selected spectrum at the top of the display.

Adding Text to the Spectrum Display

To add text labels to the spectrum display, click . When selected, the Text toolbar button changes color to show that it is active. Move the mouse to where you want to position text and left-click to open the Edit Text String dialog.



Enter the text in the Text field, select desired options and click **OK**. You can change the position of the user text by dragging it to a new position. Use the handles at the sides or corners of the text box to size the text. If you want to edit the text, double-click it to redisplay the Edit Text String dialog.

The font and color of the user text can be changed in the **Colors and Fonts** option on the TurboMass **Tools** menu. Any changes made to fonts or colors will only apply to text added after the changes. If you want to change existing text, you must delete and reinsert it. Other formatting options available for user text are as follows.

Justification Text can be aligned to the left, right, or center of the text area.

Border If selected, draws a box around the user text.

Vertical If selected, displays text vertically rather than horizontally.

Autosize If selected, causes the text area to be initially defined just large enough to hold the user text. If not selected, two boxes will appear on the display. You must select one of them, and drag until text area is the required size.

Attach to Axis If selected, text can only be positioned within a box defined by the intensity and time/scan axes. If not selected, text can be positioned anywhere on the display.

Processing Spectra

The following procedures describe how to manipulate processed spectra data.

Saving and Recalling Processed Spectra

The spectra resulting from any spectral processing can be saved with the raw data.

Saving a processed spectrum

1. Select the processed spectrum in the Spectrum window, and select **Save Spectrum** from the Spectrum **File** menu.

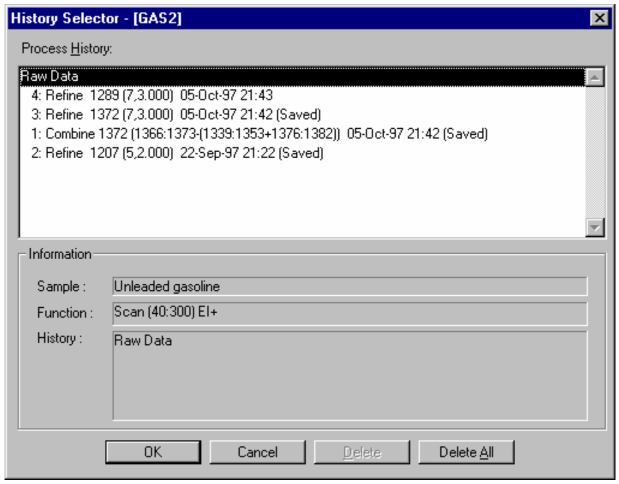
   The Spectrum Save dialog will be displayed giving a brief description of the process you want to save

2. Click **OK** to save the process and exit.

Reloading processed data into Spectrum

1. Click **Open** from the Spectrum **File** menu.

2. Select the raw data file from which the processed data were obtained, and click **History** to open the History Selector dialog.



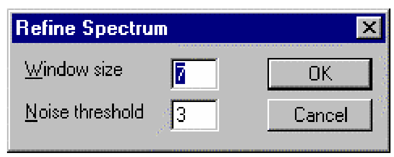
3. From the **Process History** list, select the processed data you want to load.

4. Click **OK** to exit the History Selector dialog.

5. Click **OK** to exit the Data Browser and open the processed data.

Refine

The refine process operates on centroid-mode data only. Its purpose is to identify just those masses that contribute to a specific peak in the TIC.



You identify a particular TIC peak by specifying the peak top scan. You supply two parameters for the process: window size (based on GC peak width n scans) and noise threshold.

The refine algorithm proceeds by generating the summed mass chromatogram over a range of 1 Da centered on each integer mass in turn. It examines these chromatograms for a number of scans equal to the window size around the peak top scan. If there is a

peak present in this range whose topmost point is within one scan of the peak top scan and more intense than the noise threshold value, then this mass will appear in the refined spectrum. Note that it is very important to be on the peak apex when using this function.

Refine is a good alternative to background subtraction (Combine) when performing library searches or selecting spectra for a Quantify method.

To refine a scan in a centroid-mode data file

1. Identify the scan at the top of the peak you are interested in. Display this scan in a spectrum window by double-clicking the chromatogram peak.

Choose Refine from the Spectrum Process menu. Enter values for Window size and Noise threshold. Window size is the half width in scans at baseline of the TIC peak of interest. For the first run, set Noise threshold to zero to show all peaks.

Choose OK.

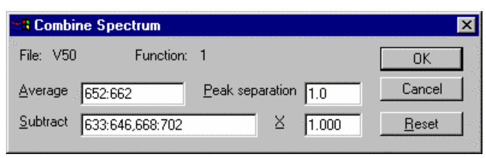
If the noise level in the refined spectrum is unacceptable, repeat the refine operation with a higher Noise threshold setting. Values in the range 0-10 are recommended.

OR

- Refine the current spectrum using the current refine parameters by choosing  on the Spectrum toolbar.

Combine

The combine process operates on centroid-mode or continuum data. Its purpose is to produce a single scan from all the scans across a TIC peak. The combined scan exhibits enhanced signal-to-noise and improved mass accuracy.



You specify three scan ranges and a background factor. One range contains the scans across the peak top and the other two ranges contain scans from the background, on each side of the peak. The scans across the peak top are averaged together and the average of all the background scans, multiplied by the background factor (X), is subtracted from the result.

Peak separation is the spectral peak width in Da. For centroided data the peak width can be determined from inspection of the tune peaks on the Tune page. The Combine algorithm combines peaks within a **Peak separation** window into a single peak. Clicking **Reset** will remove all values that have been entered into the dialog.

Combining scans in a centroid-mode data file

1. Display the chromatogram peak of interest in a chromatogram window.
2. Select **Combine** from the Spectrum **Process** menu.
3. Enter the peak top scan range either by entering scan numbers separated by a colon (for example, 619:626) into the **Average** field, or by right-clicking dragging the mouse across the peak.
4. Optionally, enter one or two background scan ranges. Again, you can do this either by entering scan numbers into the **Subtract** field, or by right-clicking and dragging the mouse. If you enter the values, each range should be in the form of two numbers separated by a colon, as above; and, if there are two ranges, they should be separated by a comma (for example, 606:612,631:637). If you use the mouse, right-click and drag the mouse across the first background scan range; then optionally repeat for a second range.
5. Optionally, enter a background factor in the **X** field.
6. Optionally, enter a **Peak separation** value.
7. Click **OK**.

Subtract

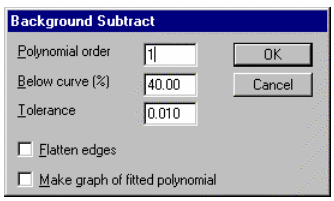
Background Subtract adjusts the zero level in a continuum spectrum to lessen the effect of chemical noise caused, for example, by column bleed. A low order polynomial is fitted to the data to remove a constant, sloping, or curved background from a spectrum.

The algorithm fits a polynomial of specified order (zero is a flat baseline, one is a straight, sloping line, two is a quadratic shape, etc.) to a spectrum such that a specified percentage (usually 30 % - 50 %) of the data points in the spectrum lie below the polynomial. This operation is performed to an arithmetical tolerance that you specify.

The Background Subtract process also gives you the option to display a graph of the baseline, which will be fitted to the data before doing the Background Subtraction.

Subtracting the background from a continuum spectrum

1. Select **Subtract** from the Spectrum **Process** menu to open the Background Subtract dialog.



2. Set the **Polynomial order** parameter to 0 for a flat baseline, 1 for a sloping straight baseline, or 5 for a curved baseline.

3. If desired, the **Below curve (%)** parameter can be changed from its default value of 40 %. The effect of increasing this parameter is to raise the zero level in the spectrum. Half the noise lies above the zero line, and half below. Therefore half of 80 %, or 40 % of the total number of data points, should lie below the background zero level.

4. If desired, you can change the **Tolerance** parameter from its default value of 0.01. Increasing this parameter causes the algorithm to terminate sooner, but the result may not be as good.

5. If you want to see what the effect of this Background Subtraction would be on the data before actually performing the run, select **Make a graph of fitted polynomial** and click **OK**.

   TurboMass displays a graph of the polynomial function that would be subtracted from the spectrum above the resulting subtracted spectrum.

   If you select **Link Vertical Axes** and **Overlay Graphs** from the Spectrum Display dialog, the new baseline will be superimposed on the existing data.

6. When you are satisfied with the parameters, deselect **Make a graph of fitted polynomial**.

7. Click **OK**.

   The Background Subtract dialog indicates the progress of the subtract algorithm. After every iteration, the convergence value in the dialog is updated. The algorithm terminates when convergence is less than tolerance.

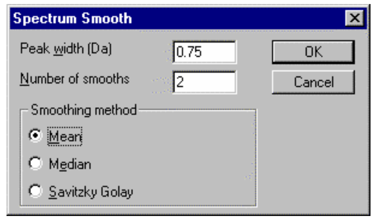
   Select the appropriate parameters in the Spectrum Display dialog to choose whether to view the zero level and negative data in the spectrum.

   When **Flatten edges** is selected, TurboMass verifies that the polynomial applied is flat or horizontal at the beginning and end of the trace.

Smooth

Smoothing reduces the high-frequency noise present in a spectrum, thus aiding interpretation. We strongly recommend that you smooth data before attempting mass measurement with the Center process; otherwise peaks may result from the noise spikes.

Three types of smoothing are available in TurboMass: **Mean**, **Median**, and **Savitzky Golay**. The most generally useful technique is **Mean**. Using **Savitzky Golay** smoothing will allow you to use a heavier smooth without broadening the peak as much. **Median** is used for removing noise spikes that are much narrower than actual real peaks (for example, single ions, electronic spikes).



All three methods slide a window along the data, averaging the data in the window to produce a point in the smoothed spectrum. The width of the smoothing window in data points is determined by the data system using the equation:

$$\textit{Halfwidth of smoothing window} = \frac{\textit{Full peak width at 50\% intensity}}{3\delta m}$$

Where δm is the spacing between adjacent points on the mass axis, for example, 0.0625 Da for raw continuum/MCA data.

Mean takes the arithmetical mean of the intensities of the data points in the window.

Savitzky Golay takes an average of the intensities weighted by a quadratic curve, which tends to enhance quadratic-shaped features in the data (peaks!).

Median takes the arithmetical median of the intensities of the data points in the window. This process is unlike the previous two in that the median smooth iterates until the spectrum no longer changes. The effect is that the intensity of narrow spikes is reduced on successive iterations, to background level on convergence.

Smoothing a continuum spectrum

1. Expand a section of the spectrum sufficiently to allow you to estimate the width of a peak at half height.

2. Select **Smooth** from the Spectrum **Process** menu.

3. Set **Peak width (Da)** according to the value you estimated in step 1.

4. Select a smoothing method.

If you have selected **Mean** or **Savitzky Golay**, you may want to alter the number of times the smooth is repeated by changing the **Number of smooths** parameter from its default value of 2. Increasing this parameter gives a heavier smooth.

NOTE: *This parameter has no effect on* **Median** *smoothing, which always iterates until the spectrum is unchanged.*

5. Click **OK**.

   The **Median** smoothing algorithm has the side effect of producing peaks with flattened tops. For this reason, it is recommended that you follow a **Median** smooth with a single iteration of a **Mean** or **Savitzky Golay** smooth.

Center

Peak centering uses all the points across a peak in a continuum trace to calculate the mass of the peak center.

You can use the centering process to either label each peak with the calculated mass, or to produce a single stick from each peak in a continuum spectrum. The calculation can be performed in three ways:

- Select the most intense (top) point on the peak.
- Calculate the centroid of the peak. This is equivalent to finding the vertical line passing through the center of gravity of the peak. This will provide a more accurate mass measurement, unless the peak contains a coeluting compound.
- Calculate the median of peak area. This is equivalent to drawing the vertical line such that half the area of the peak lies on either side.

There is little practical difference between the median and centroid methods, though it may be the case that the median is a more robust statistic on very asymmetric peak shapes. You should not compare masses from different experiments obtained by centering with different methods.

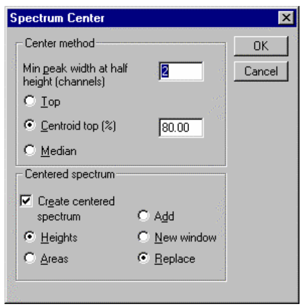
The centering algorithm looks for the trace rising then falling to indicate the top of a peak. You specify how many data points must be visible as a clear peak top before the algorithm turns the peak into a stick.

For the centroid method, you also have the option of using only a specified fraction of the resolved part of the peak. This will help to avoid the mass given to the stick being affected by unresolved neighboring peaks.

Centering a continuum spectrum

1. First background subtract, then smooth the spectrum. Background subtraction will tell the centering algorithm how much of the spectrum is noise, and therefore reduce the amount of noise seen in the resultant stick spectrum. Smoothing will help the centering algorithm make sensible decisions about whether groups of data points represent peaks, or noise spikes.

2. Select **Center** from the Spectrum **Process** menu to open the Spectrum Center dialog.



3. The **Min peak width at half height (channels)** parameter determines how many data points must be visible in the expected shape across the peak top, that is, minimum width. For continuum/MCA data, setting this parameter to 4 is safe. As there are 16 data points collected per Dalton, the value 4 is equivalent to 0.25 Da.

   Too low a setting of the peak width parameter will result in the centering algorithm producing sticks from the high-frequency noise.

   Too high a setting of the peak width parameter will result in the centering algorithm misinterpreting many peaks to produce a single stick.

4. Select a centering method.

5. If you have selected **Centroid top (%)**, you may want to alter the fraction of the resolved portion of the peak that is used to calculate the centroid from its default value of 80 %. Values in the range 60 % - 95 % are reasonable.

6. If you want to generate a stick spectrum, select **Create centered spectrum**. The height of the sticks can either represent the intensity of the continuum trace at the mass of the stick (select **Heights**), or the sum of the intensities of the points across the peak in the continuum trace (select **Areas**). The stick spectrum can be added to the current spectrum window, replaced with the current spectrum, or be placed in a new window.

7. Select **Add**, **Replace**, or **New window**, as appropriate.

8. Click **OK**.

Copying to and from the Windows Clipboard

The Windows Clipboard provides temporary storage for information that is being transferred between application programs (word processors, spreadsheets, TurboMass etc.). You can use the Clipboard to move data in or out of the Spectrum window, either as a picture or as a text list. For example, you can paste spectra or chromatograms into reports written with a Windows compatible word processor.

TurboMass can copy a Spectrum picture to the Clipboard as a metafile giving greatly improved resolution. When the metafile is pasted into another windows application it can be rescaled if required without distorting the original image as long as the original aspect ratio is maintained. When you use the TurboMass Edit Copy Picture command both a metafile and a bitmap are copied to the Windows Clipboard.

Copying a spectrum as a picture to the Clipboard

1. Produce the required display in a Spectrum window.

2. Click 

   OR

   Select **Copy Picture** from the Spectrum **Edit** menu to copy the contents of the window to the Clipboard as both a metafile and a bitmap.

3. To read the image into another application as a metafile, select **Paste** from the other application's **Edit** menu. If you select **Paste Special** from the other application's **Edit** menu, you will be given the option of pasting either the metafile or the bitmap.

Copying a spectrum as a text list to the Clipboard

1. Display the required mass range in a Spectrum window.

2. Click 

   OR

   Select **Copy Spectrum List** from the Spectrum **Edit** menu. The section of the spectrum on display will be transferred to the Clipboard as (mass, intensity) pairs.

3. To read the information into another application, select **Paste** from the other application's **Edit** menu.

Pasting information into a spectrum window from the Windows Clipboard

1. Click 

   OR

   Select **Paste** from the Spectrum **Edit** menu to paste the default Clipboard object to Spectrum.

2. Select **Paste Special** to choose which object to paste into Spectrum. These objects would typically be metafiles, bitmaps, or text.

3. Use the mouse to move the outline of the image to the required position.

   You can paste the contents of the Clipboard, (whether a bitmap, a metafile, or text,) into a spectrum window. If in textual or metafile form, you can rescale data using the mouse and there will be no distortion of the image. However if you paste a bitmap, rescaling is done by stretching the image, which will cause some distortion. To avoid this, scale the image to the required size before you copy it to the Clipboard.

Removing pasted input from the display

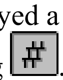
1. Left-click to select the item you want to remove.

2. Press DELETE.

Manipulating Library Spectra

Displaying a library entry

1. Select **Get Spectrum** from the Spectrum **Edit Library** menu.
2. If required, select a new library by clicking **File**.
3. Enter an entry number in the **Entry** field.
4. You can add the library spectrum to the current spectrum window, replace the current spectrum, or be placed the library spectrum in a new window. Click **Add**, **Replace** or **New**, as appropriate.
5. Click **OK**.

   Once you have displayed a spectrum from a library, you can browse the rest of the library by clicking .

Appending the current spectrum to the current library

1. Select **Append** from the Spectrum **Edit Library** menu.
2. Click **OK**.

Adding the current spectrum to a new library

1. Select **Append** from the Spectrum **Edit Library** menu.
2. Click **File**.
3. Enter the name of the user library to be created for File Name.
4. Click **Open**.
5. Click **OK**.

NOTE: *For this spectrum to be used for library searching it first must be processed by Index Library in the Library* **Search Process** *menu.*

Strip and Combine Functions 15

Strip Functions

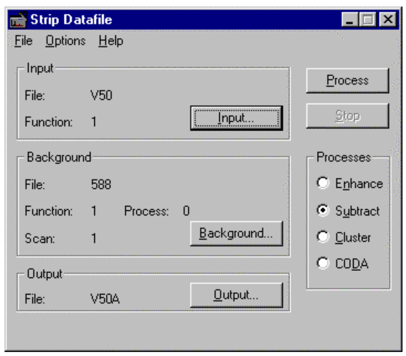
The Strip application removes unwanted background and noise from a data file. Processing a data file using Strip creates a new file that is stored in the same format as a raw data file and can be displayed and processed in the same way as a raw data file. The original input file is retained unmodified.

Opening the Strip application

➢ Select **Strip** from the TurboMass top level **Tools** menu

OR

Click  to open the Strip Datafile dialog.



NOTE: *The* **Strip** *application cannot be accessed while the* **Combine Functions** *application is opened. Likewise, the* **Combine Functions** *application cannot be accessed while the* **Strip** *application is opened.*

Strip provides four processing options: **Subtract**, **Enhance**, **Cluster**, and **CODA**.

Subtract Can subtract either a single background spectrum or a whole data file from the input file. Processed spectra can be subtracted, enabling averaged spectra to be used as background. Both centroid and continuum type files can be subtracted; different

types cannot be mixed.

Enhance Removes noise from continuum data files. It examines each data point, and its close neighbors, to determine if it is noise or part of a real feature. Data points not considered to be valid are removed from the output data file. **Enhance** can significantly reduce data file size.

Cluster Detects pairs or triplets of peaks separated by a specified mass difference. Parameters specified are mass differences and expected intensity ratios, both with tolerances, together with a time window and a global threshold. The resulting data file will contain only these peaks. Again, **Cluster** will significantly reduce data file size.

CODA (COmponent Detection Algorithm) essentially removes mass chromatograms that represent background from the dataset. Each raw mass chromatogram is compared to a smoothed, standardized mass chromatogram, and masses in which the background is high or in which spikes are present are rejected.

Creating a Subtracted Data File

The following section describes how to create a subtracted data file and provides examples.

1. Select **Subtract** in the Strip Datafile dialog.

2. To change **Input File** or to select a subrange, click **Input**. Select **Input File** and **Function** by clicking **File** to open a browser dialog. Set the **Mass** and **Retention Time** ranges if required.

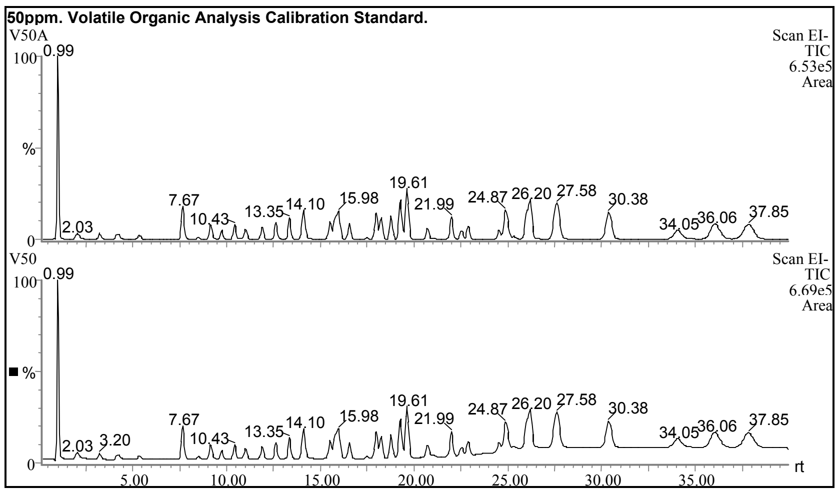
3. To change **Background File** or **Scan** number, click **Background**. Select the **Input File** and **Function** by clicking **File**. Enter **Background scan** number or select **Use all background file** if the entire file is to be used. If a previously generated spectrum process is to be used, click **File** to open the browser, and click **History** within the browser.

4. If the default **Output** file name is not correct, click **Output** and enter the required name.

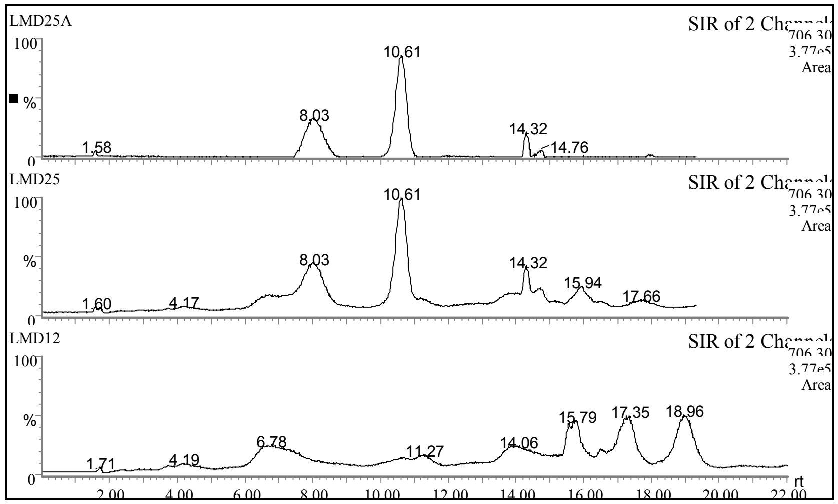
5. Set the Subtract parameters by selecting **Subtract Datafile Options** from the Strip **Options** menu.

6. Click **Process** to start processing the data file. The status bar at the bottom of the Strip dialog displays the progress of the current process.

The lower trace shows the TIC chromatogram of the V50 data file. The upper trace shows the TIC chromatogram of the same data file after a background scan (scan 761 at retention time 32 min) has been subtracted.



The illustration shows an example of subtracting a complete data file from another data file. The lower trace shows a mass chromatogram from the blank sample, the middle trace shows a mass chromatogram from the analyte sample, and the upper trace shows the result of subtracting the blank data file from the analyte data file.


LMD25A
SIR of 2 Channels
706.30
3.77e5
Area
100
%
0
1.58
8.03
10.61
14.32
14.76
LMD25
SIR of 2 Channels
706.30
3.77e5
Area
100
%
0
1.60
4.17
8.03
10.61
14.32
15.94
17.66
LMD12
SIR of 2 Channels
706.30
3.77e5
Area
100
%
0
1.71
4.19
6.78
11.27
14.06
15.79
17.35
18.96
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
rt

Creating an Enhanced Data File

This section describes how to create an enhanced data file and provides examples.

1. Select **Enhance** in the Strip Datafile dialog.

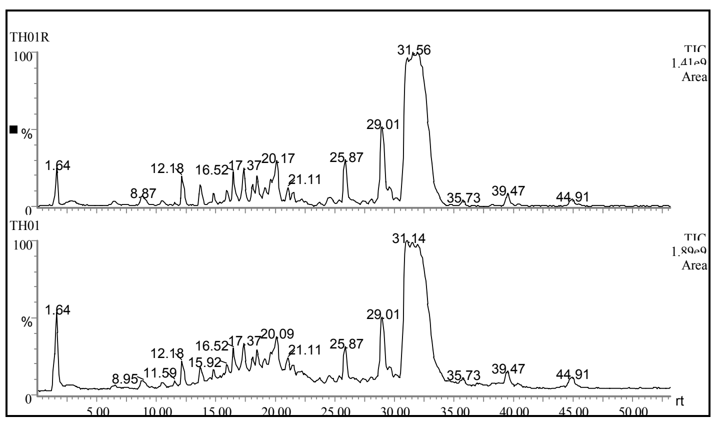
2. To change **Input File** or to select a subrange, click **Input**. Select the input file and function by selecting **File** to open a browser dialog. Set the mass and retention time ranges if required.

3. If the default Output file name is not correct, click **Output** and enter the required name.

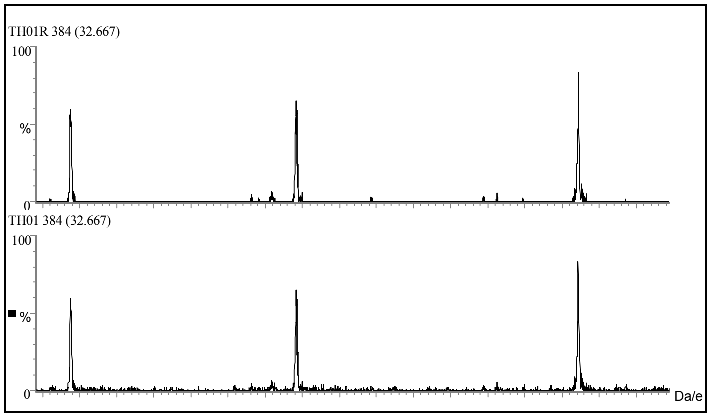
4. Select **Enhance Datafile Options** from the Strip **Options** menu to set the Enhance parameters.

5. Click **Process** to start processing the data file. The status bar at the bottom of the Strip dialog displays the progress of the current process.

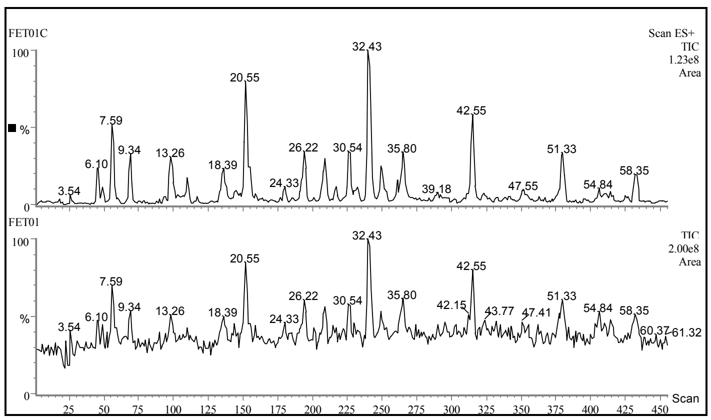
The following illustration shows two chromatogram traces. The lower trace is the raw data file. The upper trace shows the same data file after it has been processed using Enhance. As you can see the background noise level has been greatly reduced in the enhanced data. The original data file size of 19 MB has been reduced to 0.5 MB in the enhanced data file.



The following illustration shows part of a single scan from the raw and enhanced data files. The background noise in the enhanced spectrum has been greatly reduced.



In the following illustration the lower trace is the raw data file, the upper trace shows the same data file after it has been processed using Enhance to reduce background noise. The original data file size of 41.2 MB has been reduced to 1.4 MB in the enhanced data file.



Creating a Clustered Data File

The following describes how to create a clustered data file and provides examples.

1. Select **Cluster** in the Strip Datafile dialog.

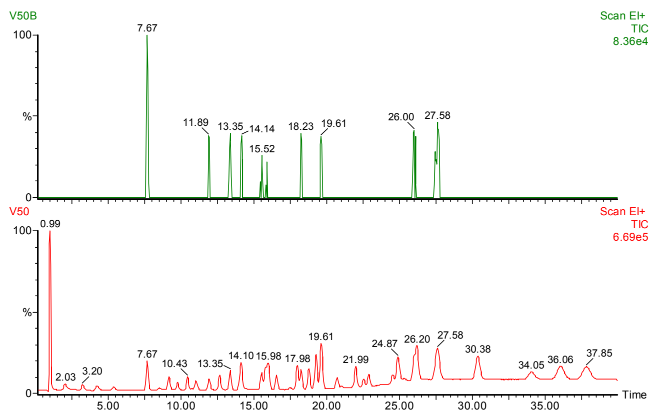
2. To change **Input File** or to select a subrange, click **Input**. Select input file and function using by choosing **File** to open a browser dialog. Set the mass and retention time ranges if required.

3. If the default **Output** file name is not correct, click **Output** and enter the required name.

4. Select **Cluster Datafile Options** from the Strip **Options** menu to set the Cluster options.

5. Click **Process** to start processing the data file. The status bar at the bottom of the Strip dialog displays the progress of the current process.

The illustration shows the spectrum of a mixture of chlorinated and non-chlorinated compounds. The lower trace is the raw data file, the upper trace shows the same data file after it has been processed using the Cluster option to show pairs of peaks differing in mass by 2 Da. The illustration shows the spectrum of a mixture of chlorinated and non-chlorinated compounds.



Creating a CODA Data File

The following describes how to create a CODA data file and provides examples.

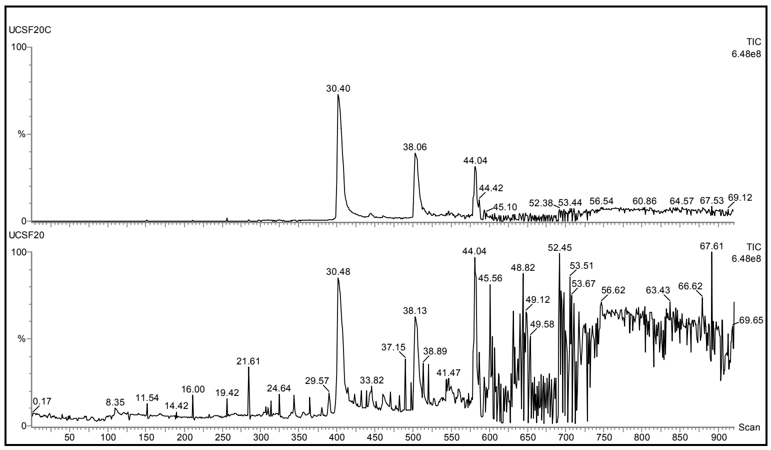
1. Select **CODA** in the Strip Datafile dialog.

2. To change **Input File**, click **Input** to open a browser dialog. Note that input mass range cannot be changed and all functions are processed irrespective of function selected.

3. If the default **Output File** name is not correct, click **Output** and enter the required name.

4. Select **CODA Options** from the Strip **Options** menu to set the CODA options.

5. Click **Process** to start processing the data file. The status bar at the bottom of the Strip dialog displays the progress of the current process.



Selecting a Data File to Process

➢ The **Input** section of the Strip Datafile dialog identifies the data file and function number that will be processed.

Changing the current input file

➢ Select **Input** from the Strip **File** menu to open a Datafile Browser dialog from which a new file, function, and directory can be selected.

By default, TurboMass will process the entire selected function.

Selecting a new input file automatically defaults the name of the output file.

Selecting a Data File and Subrange to Process

NOTE: *CODA does not allow subrange selection. This is because all functions in the dataset are processed.*

Processing a mass or retention time subrange of the input file has the advantages of reducing both processing time and the size of the resulting output file.

Selecting a different file and function

1. Select **File** to open the Strip Data Browser dialog.

2. Selecting a new file automatically defaults mass and retention time to full range.

3. Enter values for the **Mass Range** and **Retention Time** range that you wish to process.

   These ranges can be set from Spectrum and Chromatogram respectively, by right-clicking and selecting the desired range.

4. To set the **Mass Range** parameters, right-click at one end of the Spectrum region of interest, and drag the mouse horizontally to the other end. TurboMass indicates the range you have selected. The Input Datafile dialog will be updated to show the new mass range.

5. To set the **Retention Time** parameters, right-click at one end of the Chromatogram region of interest, and drag the mouse horizontally to the other end. TurboMass indicates the range you have selected. The Input Datafile dialog will be updated to show the new retention time range.

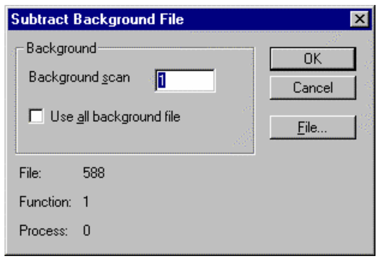
6. Click **Default** to set both mass and retention time to the full range of the current file.

Selecting a Background Data File

The **Background** section of the Strip Datafile dialog identifies the data file, function, and scan number to be used as background when performing the Subtract process. Previously processed spectra can be used as background. The background file is not used for Enhance processing.

Subtracting a background file

1. Click **Background** in the Strip Datafile dialog to open the Subtract Background File dialog.



2. To select a different file and function, click **File** to open the Strip Data Browser.

3. A previously processed spectrum can be selected by clicking **Browser History**. Selecting a new file automatically defaults to the first scan in the data file.

4. If a single background scan is to be subtracted, enter the scan number in the **Background scan** field. The scan number can also be set from Spectrum and Chromatogram by right-clicking and selecting the desired scan.

   If Background scan is deselected, deselect Use all background file.

5. To subtract the entire background file, select **Use all background file**. In this case, the background scan with the closest retention time to each input scan will be subtracted.

Selecting an Output Data File

The **Output** section of the Strip Datafile dialog identifies the data file that will be created by Strip when processing.

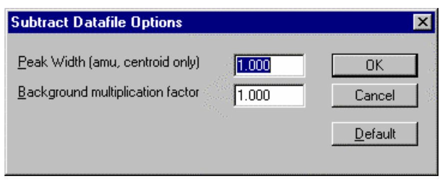
When an **Input** File is selected, the **Output** File defaults to the same directory and a name based upon the Input name with an extra letter appended. For example, if the input file was \turbomass\data\v50.raw the default output file might be \turbomass\data\v50a.raw. When defaulting the output name, TurboMass attempts to choose a name that does not already exist.

Changing the default output file and directory

1. Click **Output** in the Strip Datafile dialog to display the Output File dialog.
2. Enter a name for the output file.
   To change the directory of the file, enter the full path name of the file.

Setting Subtract Datafile options

1. Select **Subtract Datafile Options** from the Strip **Options** menu to display the Subtract Datafile Options dialog, and enter the appropriate values.



Peak Width	This parameter is the spectral peak width in amu. It is only used when subtracting centroid data. The peak width can be determined from inspection of the tune peaks on the Tune page. The peak width is used to determine if peaks present in the input and background data represent the same peak.
Background multiplication factor	This is applied to the intensities of the peaks in the background spectra before they are subtracted from peaks in the input spectra. This provides a method of adjusting the height of the subtracted background.

2. To set parameters to their default values, click **Default**.

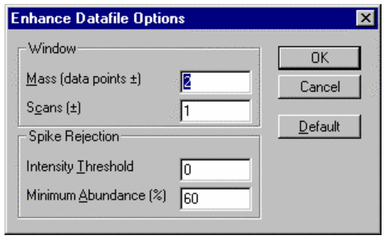
Setting Enhance Datafile Options

Enhance operates on continuum data only. It works by examining each spectrum data sample to determine if it is a noise spike or part of an actual peak. This is achieved by looking at neighboring samples on the mass scale and at the same area in the preceding and following scans.

For example, using the values in the Enhance Datafile Options dialog, two samples either side of the current sample will be examined, including the current sample. This makes five in all. One scan either side of the current scan will be used, so including the current scan three scans will be used. Multiplying the number of scans by the number of samples in each scan shows 15 samples are examined in all. Consequently for a sample to be accepted 60 % of these samples (nine samples) must have an intensity greater than the specified **Intensity Threshold**.

Setting the Enhance processing parameters

1. Select Enhance Datafile Options from the Strip Options menu.



2. Set the following parameters as required.

Mass (data points ±)	Determines how many samples to look backwards and forwards along the mass scale. The Mass parameter should not exceed half the number of samples that make up a peak.
Scans (±)	Determines how many scans to look backwards and forwards, respectively. It should not exceed half the number of scans a chromatogram peak is present.
Intensity Threshold	Defines an absolute intensity that a data point must exceed to be regarded as being significant. For spectra with a high baseline, this parameter will need adjusting so that its value is approximately equal to the intensity at the top of the noise. The larger this value the more likely that information will be discarded as being noise.
Minimum Abundance (%)	Determines the minimum percentage of neighboring samples examined whose intensity must be above the specified threshold for the current sample not to be rejected as noise. The larger this value the more likely that a sample will be discarded.

3. To set the parameters to their default values, click **Default**.

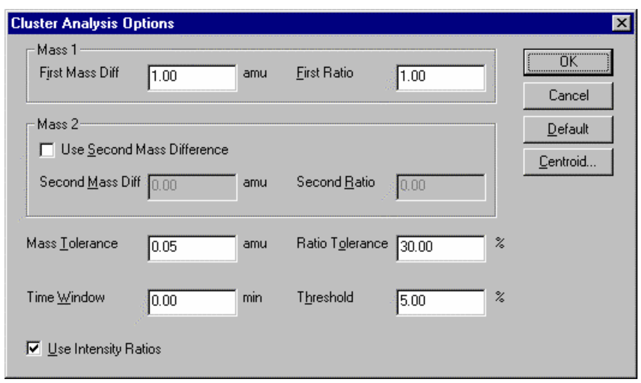
Setting Cluster Datafile Options

Cluster operates on both centroid and continuum data. For continuum data, a special fast centroid process is used. See *Setting Cluster Centroid Options* on page 478. The centroid process works by examining each pair (or triple) of peaks in each spectrum to determine if they are separated by the correct mass difference(s) and if their intensity ratios lie in the correct range(s). If **Time Window** is set to a value other than zero, then neighboring scans within that time window (+/-) are examined.

For example, using the values in the Cluster Analysis Options dialog; mass difference 1 22.0 Da, mass difference 2 33.0 Da, both intensity ratios 1.0, mass tolerance 0.5 Da, ratio tolerance 30 %, time window 0.00 min, threshold 0.01 %. Triplets will be detected, with the mass difference between the first two peaks being 21.5-22.5 Da, and between the first and third peaks 31.5 - 32.5 Da. The intensity ratios of the peaks must lie in the range 0.7 to 1.3 (low mass peak / high mass peak), and the peaks must lie in the same scan. The peaks must be more intense than 0.01 % times the most intense peak in the function.

Setting Cluster processing parameters

1. Select **Cluster Datafile Options** from the Strip **Options** menu to open the Cluster Analysis Options dialog.



2. Set the following parameters as required

First Mass Diff and **First Ratio**	Determines the requested separation and intensity ratio of the first pair of peaks. The intensity ratio is calculated as (intensity of low mass peak) / (intensity of high mass peak). The requested intensity ratio may be less than 1. Intensity ratio comparison may be deselected using **Use Intensity Ratios**; if not selected, then no ratio comparison is attempted, and peaks are selected purely on the basis of mass difference.
Second Mass Diff and **Second Ratio**	Determines the mass difference between, and intensity ratio of, the first and third peaks in the triplet; note, not the first and second. The second mass difference can be calculated by selecting **Use Second Mass Diff**; if not selected, then examination is restricted to pairs of peaks only, not triples.
Mass Tolerance	Specifies a window (+/-) for each of the (maximum of two) specified mass differences. Pairs or triples of peaks are detected if the corresponding peak(s) lay at the specified mass difference +/- the specified mass tolerance.
Ratio Tolerance	Specifies the maximum mismatch between specified and calculated intensity ratios. It is specified as a percentage of the intensity ratio(s).
Time Window	Determines how far apart scans may lie in which peaks forming part of the pair/triple are located. For instance, if time window is +/- 0.5 min, with mass difference 5.0 amu, then a peak at mass 25.0 Da in a scan at time 2.2 min will match with a peak at mass 30.0 Da in a scan at time 2.7 min.

Threshold	Defines an absolute intensity that a data point must exceed to be regarded as being significant. For spectra with a high baseline this parameter will need adjusting so that its value is approximately equal to the intensity at the top of the noise. The larger this value the more likely that information will be discarded as being noise.

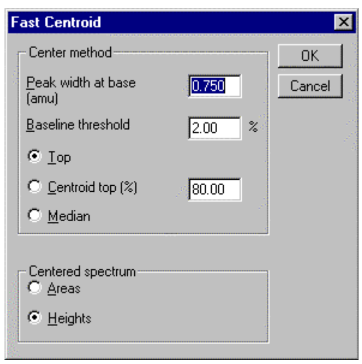
3. Click **Default** to set the parameters to their default values.

Setting Cluster Centroid Options

The Fast Centroid process is unique to the cluster algorithm. It was developed to reduce the time taken to centroid each scan of a run. Consequently, it will not deal as accurately with multiplets as the standard centroid algorithm, but should be perfectly adequate for most applications.

Setting the Cluster Centroid processing parameters

1. From the Cluster Analysis Options dialog, click **Centroid** to open the Fast Centroid dialog.



2. Set the following parameters, and click **OK**.

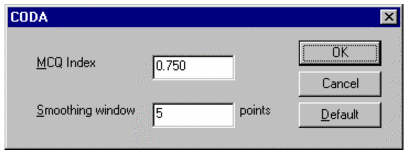
Peak width at base (amu)	Specifies the expected width of the continuum peaks at baseline. It has two purposes; first, it determines the amount of smoothing that is applied to the continuum spectrum prior to centroiding proper, and second it determines how close together two sticks must lie in order to be grouped into a single stick, that is, it controls the multiplet resolution. For smoothing, the width at half height of the peak is estimated as half the specified width at baseline, and it is this estimated value that is used in the smooth. For multiplet resolution, peaks closer than the specified **Peak width at base** distance together will be regarded as a singlet.
Baseline threshold	Specifies the minimum signal level in the spectrum above which a peak will be considered significant.
Top, Centroid, Median	These parameters allow a selection of peak **Top**, peak **Centroid**, and peak **Median** methods to be made. This functions as for the standard centroid software (see *Center* on page 453). Similarly, selection of peak areas or heights is the same as in Spectrum.

Setting CODA Options

CODA operates on both centroid and continuum data. It works by standardizing and smoothing each mass chromatogram in the dataset, and then comparing the smoothed, standardized mass chromatogram with the raw chromatogram. If they are sufficiently similar, as determined by the MCQ Index parameter, then the mass chromatogram is preserved; otherwise, it is removed. Essentially, mass chromatograms that contain spikes or are noisy will be dissimilar after smoothing and standardization to the raw mass chromatogram and are hence rejected.

Setting the CODA processing parameters

1. Select **CODA Options** from the Strip **Options** menu to open the CODA dialog.



2. Set the following parameters, and click **OK.**

MCQ Index	Specifies how similar the smoothed, standardized mass chromatogram must be to the raw mass chromatogram before it is preserved. The parameter is in the range 0 - 1 inclusive; a value of 0 will preserve all mass chromatograms and result in the raw file being copied to the output. A value of 1 will result in all mass chromatograms being rejected, and an empty file. Values around the default value of 0.75 are most useful, with the range 0.65 - 0.85 recommended.
Smoothing window	Specifies the amount of smoothing given to raw mass chromatograms. The default value of 5 is usually adequate. This window is (+/-) a number of data points around the central point.

Stopping a Process

When you stop a process before completion, the output data file will contain all the information written up to the point at which the process was stopped.

➢ Click **Stop** in the Strip Datafile dialog.

Confirmation of the action will be requested.

Combine Functions

The Combine Functions application provides a way of combining all functions in a data file to produce a new data file containing a single function, which is the sum of the multiple functions. The Combine Functions option is particularly useful for combining functions acquired with CI+ and CI- in the same chromatogram.

To use the Combine Functions option, all the functions in the data file must have been acquired using the same scan range and scan rate, or must contain the same SIR ions.

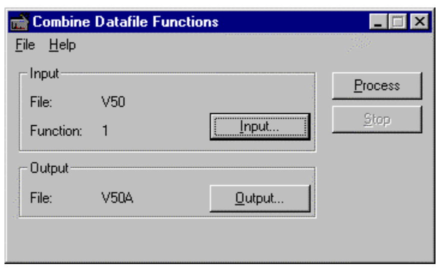
NOTE: *The Combine Functions application cannot be accessed while the Strip application is opened. Likewise, the Strip application cannot be accessed while the Combine Functions application is opened.*

Creating a Combined Datafile

1. Select **Combine Functions** from the TurboMass top level **Tools** menu

   OR

   Click  to open the Combine Datafile Functions dialog.

2. To change the **Input File** or to select a subrange, click **Input**. Select the input file by clicking **File** to open a browser dialog. Set the **Mass** and **Retention Time** ranges, if required.

3. If the default **Output** file name is not correct, click **Output** and enter the required name.

4. Click **Process** to start processing the data file.

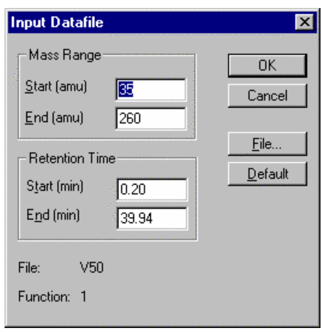
   The status bar at the bottom of the Combine Datafile Functions dialog displays the progress of the current process.

Selecting a Data File and Subrange to Process

The **Input** section of the Combine Datafile Functions dialog identifies the data file that will be processed.

Changing the current input file

1. Click **Input** from the Combine Datafile Functions dialog. This opens the Input Datafile dialog from which a new file and directory can be selected.



2. Set the parameters and click **OK**.

3. Clicking **Default** sets both **Mass Range** and **Retention Time** to the full range of the current file.

   By default, the entire selected file will be processed and all functions will be combined into a single function. To specify subranges, see below. Selecting a new input file automatically defaults the name of the output file.

   Processing a mass or retention time subrange of the input file has the advantages of reducing both processing time and the size of the resulting output file.

Selecting a different file and function

1. Click **File** to open the Combine Functions Data Browser.

   Selecting a new file automatically defaults **Mass Range** and **Retention Time** to full range.

2. Enter values for the **Mass Range** and **Retention Time** range that you wish to process.

   These ranges can be set from Spectrum and Chromatogram respectively, by right-clicking and selecting the desired range.

3. To set the **Mass Range** parameters, right-click at one end of the Spectrum region of interest and drag the mouse horizontally to the other end. TurboMass indicates the range you have selected.

   The Combine Datafile Functions, Input Datafile dialog will be updated to show the new mass range.

4. To set the **Retention Time** parameters, right-click at one end of the Chromatogram region of interest, and drag the mouse horizontally to the other end. TurboMass indicates the range you have selected.

   The Combine Datafile Functions, Input Datafile dialog will be updated to show the new retention time range.

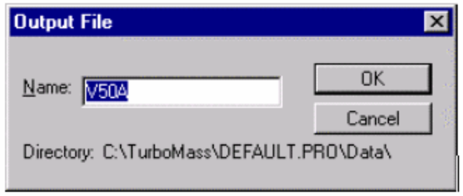
Selecting an Output Data File

The **Output** section of the Combine Datafile Functions dialog identifies the data file that will be created by Combine Functions when processing.

When an **Input** file is selected, the **Output** file defaults to the same directory and a name based upon the Input name with an extra letter appended. For example, if the input file was \mldata1\davlc7.raw, the default output file might be \mldata1\davlc7a.raw. When defaulting the output name, TurboMass attempts to choose a name that does not already exist.

Changing the default output file and directory

1. Click **Output** in the Combine Datafile Functions dialog to open the Output File dialog.



2. Enter a name for the output file.

   To change the directory of the file, enter the full path name of the file.

Stopping a Process

When you stop a process before completion, the output data file will contain all the information written up to the point at which the process was stopped.

➢ Click **Stop** in the Combine Datafile Functions dialog.

   Confirmation of the action will be requested.

Library 16

The Library application is used to identify unknown spectra by comparing the unknown spectrum to a library of known spectra. The result of a library search is a list of library compounds or "hits." The spectra in these compounds give the best match with the unknown spectrum.

This chapter describes how to search the libraries supplied, create your own mass spectral libraries, and how to use the Library Locator.

NOTE: *The terms "scan" and "spectrum" are used interchangeably in this chapter and in the TurboMass software.*

TurboMass Library Windows

The Library window presents the search results in several formats.

Hit List — Gives a text listing of the best hits. You can format the Hit List window to display a variety of information about each hit including compound name, fit values, formula, and molecular weight.

Hits Window — Shows the unknown spectrum followed by the spectra of the best hits.

Structure Window — Shows the chemical structure of the currently selected hit.

Delta Window — Shows the difference between the unknown spectrum and the spectrum of a particular hit.

Library also allows you to create your own user libraries that contain spectra from data files in the Spectrum window.

Library Editor — Used to edit libraries.

Library Locator — Used to examine a library and search for library entries that meet various criteria.

Searching a Library

The Library Search process has two parts: the Presearch and the Mainsearch. The Presearch is a faster search designed to select a number of likely candidates from the library. These candidates are then passed through to the Mainsearch, where they undergo a more rigorous and lengthy comparison. TurboMass displays the Mainsearch results in the Hit List, Hits, Structure, and Delta windows.

The Presearch

The unknown spectrum is first reduced to its eight most intense mass-weighted peaks. This reduced spectrum is then compared to the current library Presearch file. The library Presearch file contains a spectrum for each library entry that has been reduced to its eight most intense mass-weighted peaks. The Presearch process results in a list of the most likely candidates to be passed to the Mainsearch process. The most likely candidates are those compounds that have the greatest number of matching peaks with the unknown compound. You can control how many candidates are passed to the Mainsearch by changing the **Match By** parameter in the Library Search Parameters dialog.

The Mainsearch

For the Mainsearch the unknown spectrum is again reduced, this time to a number of peaks, determined by the **Sig. Peaks** parameter in the Library Search dialog.

The Search spectrum is compared to each of the possible candidates from the library, and the results of this comparison are displayed in the Hits, Hit List, Delta and Structure windows. The hits are ranked in order of best fit to the search spectrum.

You can apply various filters to the Mainsearch process to make it more specific. These filters contain requirements that must be met in order for the library entry to be included in the Hits list. These filters can contain information about the compound elemental formula and molecular weight.

TurboMass computes two types of fit values for each hit: Forward and Reverse Fit. The maximum obtainable fit value is 1,000, which represents a perfect match between the search spectrum and the library entry.

The Forward Fit value shows how likely it is that the search spectrum is a pure sample of the library entry. Any peaks that are present in the search spectrum, but not present in the library spectrum, decrease the Forward Fit value. Likewise, any peaks that are present in the library spectrum, but not present in the search spectrum, decrease the Forward Fit value.

The Reverse Fit value shows how likely it is that the search spectrum contains the library entry. In this case, the search spectrum may be a mixture of compounds. Any peaks present in the library spectrum, but not present in the search spectrum, decrease the Reverse Fit value. However peaks that are present in the search spectrum, but not present in the Library spectrum, have no effect on the Reverse Fit value.

An Overview of Library Searching

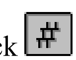
This section lists the steps in a library search. Each step is described later in this chapter.

1. Select the library or libraries that you want to search by selecting **Search List** from the Library **File** menu.

2. Select the search spectrum (scan) from the Spectrum or Library windows:

   - To select a scan from a new data file from within Library, click  or select **Open** from the Library **File** menu to open the Library Data Browser.

   OR

   - To select a new scan from the current data file, click  or select **Spectrum** from the Library **Display** menu.

3. Edit the Library search parameters by selecting **Parameters** from the Library **Edit** menu.

4. Apply any search filters by selecting **Filters** from the Library **Edit** menu.

5. Initiate the Library search from Library or Spectrum by clicking 

   OR

   Selecting **Search** from the Library **Process** menu.

6. Adjust the Library display by selecting **View** from the Library **Display** menu.

7. Format the Hit List window by selecting **Format List** from the Library **Edit** menu.

8. Print the results of the Library search by clicking  or 

   OR

   Select **Print** from the Library **File** menu.

NOTE: *All the above settings are retained for future searches and need to be edited only if you want to change them. You do not need to edit them each time you do a search.*

Library Toolbar

At the top of the Library window is a set of buttons called the library toolbar. The toolbar allows you to perform some of the most commonly used actions with the click of a button.

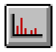
 Selects a data file.

 Prints the current window in portrait format.

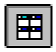
 Prints the current window in landscape format.

 Copies the bitmap of current window to the clipboard.

 Copies the current hit list to the clipboard.

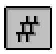
 Refines the current search spectrum.

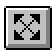
 Searches the current search spectrum against the current library.

 Arranges the windows in a tiled view.

 Arranges the windows in a cascaded view.

 Arranges the windows in a stacked view.

 Selects a new scan number as the search spectrum.

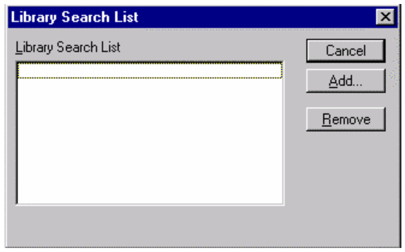
 Toggles to restore the previous display range or to display the default axis range.

Selecting Which Libraries to Search

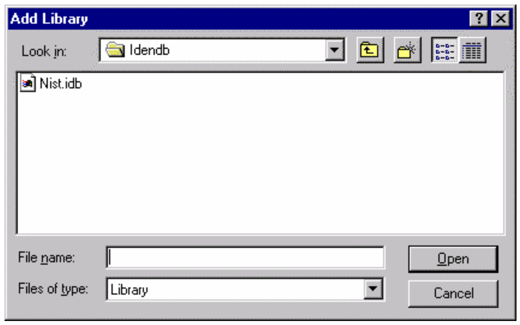
The Library application searches one or more Libraries specified in the Library Search List. These can be standard Libraries such as the NIST or Wiley libraries, or user libraries.

Building a search list

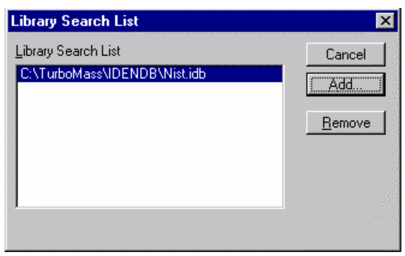
1. Select **Search List** from the Library **File** menu to open the Library Search List dialog.



2. To add a library to the search list, click **Add**.
   The Add Library dialog is displayed.



3. Select the library you want to add from the Add Library dialog, and click **Open**.
   TurboMass adds the new library to the **Library Search List**.



4. To remove a library from the search list, select file you want to remove from the **Library Search List**, and click **Remove**.

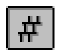
5. Click the Close button to return to the Library Hits window.

Selecting a New Search Spectrum

The spectrum currently displayed in the Library window is the current search spectrum. From the Library (Hits) window, you can select a new search spectrum (scan) from one of the following:

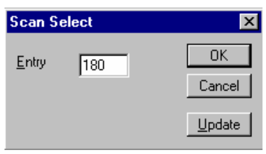
- The data file for the currently displayed spectrum (the current data file)
- A different data file
- The Spectrum window

Selecting a new search spectrum from the current data file

1. Click  from the Library toolbar

   OR

   Select **Spectrum** from the Library **Display** menu.

2. Enter the desired scan number or retention time.

   To obtain the scan number or retention time of a particular peak, click  to display the total ion chromatogram, and select **Scan** or **Time** as the horizontal axis unit from the Chromatogram **Display** menu.

3. To display the new spectrum in the Library Hits window, click **Update**.

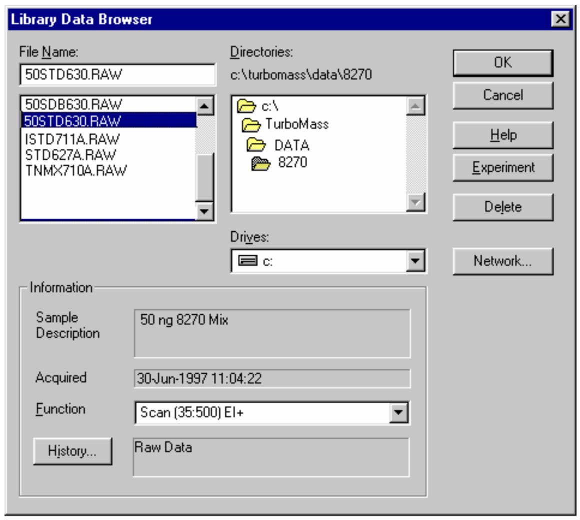
4. Click **OK**.

Selecting a new search spectrum from a different data file

1. Click 

   OR

   Select **Open** from the Library **File** menu to open the Library Data Browser dialog.



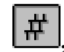
2. Select the new data file from the **File Name** list.

3. To select a processed spectrum that is the result of Combine or Refine processes, click **History**.

4. Click **OK**.

   The Hits window is updated to show Scan 1 of the new data file, which becomes the current search spectrum.

Selecting a new search spectrum from the Spectrum window

- Select a new spectrum by using the Data Browser, by clicking , or Display Spectrum.

  If you initiate the Library search from the Spectrum window, the spectrum currently displayed in the Spectrum window is used as the search spectrum. For more information, see *Spectrum* on page 423.

Setting Library Search Parameters

The Library Search parameters control how many library entries are passed from the Presearch to the Mainsearch, exactly which entries are used, and how the results are reported.

Editing the Library Search parameters

1. Select **Library** from the TurboMass **Process** menu to open the Library Hits window.

2. Select **Parameters** from the Library **Edit** menu to open the Library Search Parameters dialog.

3. Edit your library search parameters, and click **OK**.

Match By

These parameters determine how many candidates or entries are passed from the Presearch to the Mainsearch.

Level Sets the number of matching peaks that the library entry must have to be passed to the Mainsearch. You can enter a value from eight to zero matching peaks. The higher the value, the fewer entries are passed to the Mainsearch.

Viables Sets the number of matching peaks to the minimum number of entries to be passed from the Presearch to the Mainsearch. For example, if you enter a value of 8, Library first takes all entries that have eight matching peaks. If the number of entries is less than the **Viables** value, Library takes all entries that have seven matching peaks, adds these to the previous entries, and compares the new total to the **Viables** value. This process is repeated until the number of entries passed to the Mainsearch is greater than or equal to the **Viables** value. In practice, the number of entries passed to the Mainsearch is often much larger than the **Viables** value.

Sig. Peaks Determines how many spectral peaks are compared during the Mainsearch.

Exclude Masses

Masses 1-4 Allow you to exclude up to four specific masses in the search spectrum from the Mainsearch. These excluded peaks are not compared to library entries. This can be useful, for example, to exclude a contaminating ion that cannot be removed from the spectrum by any physical or chemical means.

All below Allows you to exclude all masses below a certain value.

Ranking

These parameters determine whether hits are listed in order of **Forward** or **Reverse** Fit.

Forward Indicates how likely it is that the search spectrum is a pure sample of the library entry. Any peaks present in the search spectrum, but not present in the Library spectrum, decrease the **Forward** Fit value. Likewise, any peaks present in the library spectrum, but not

present in the search spectrum, decrease the **Forward** Fit value.

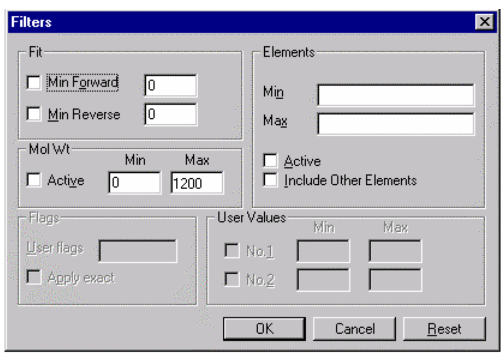
Reverse Indicates how likely it is that the search spectrum contains the library entry; in this case, the search spectrum may be a mixture of compounds. Any peaks present in the library spectrum, but not present in the search spectrum, decrease the **Reverse** Fit value. However peaks that are present in the search spectrum, but not present in the library spectrum, have no effect on the **Reverse** Fit value.

Setting Library Search Filters

Library search filters are used to specify certain criteria that a library entry must meet in order to appear in the Hit List. If you have the molecular weight and elemental formula of a compound, you can use these filters to refine the search. For example, if you know that the search compound contains at least one chlorine atom, you can specify this information in the search filters. If you know that its molecular weight falls within a certain range, you can specify this information in the search filters.

Specifying library search filters

1. Select **Filters** from the Library **Edit** menu to display the Filters dialog.



2. Change the library search filters as required by setting the following parameters.

Fit Specifies a **Minimum Forward** and/or a **Minimum Reverse**

Fit value that a library entry must have in order to appear in the Hit List. To make the filter active select the checkbox next to it and enter a value between 0 and 1000 into the relevant field.

Mol Wt These parameters specify a range within which the molecular weight of the library entry must fall in order to be included in the Hit List.

Active To make the filter active, select **Active** and enter the minimum and maximum molecular weights in the **Min** and **Max** fields.

Min and **Max** Specifies the minimum or maximum molecular weight that an element must have for its entry to appear in the Hit List.
To specify a particular molecular weight, enter equal **Min** and **Max** values.

Elements These parameters specify the number of particular elements that must be present in the library entry molecular formula in order for the entry to appear in the Hit List.

Min Specifies the minimum number of elements that must be present in an entry in order for it to appear in the Hit List.

Max Specifies the maximum number of elements that must be present in an entry in order for it to appear in the Hit List.

Active To activate the filter specified in the **Max/Min** fields, select the **Active** checkbox.
Enter elemental formulas in the “standard” format as an element symbol, followed immediately by its count, if greater than unity, and then immediately by another symbol, as relevant.
For example, suppose you want to set the **Elements** parameter to C6H20NClBr2. Enter symbols in the standard upper and lower case format. Note that "Cl" does not need a "1" after it and that there are no spaces. The specific order of elements is

irrelevant.
If you have a specific formula to match, enter this formula in both the **Min** and **Max** fields, and do not select **Include Other Elements**.
If an element appears only in the **Min** field, there is no upper limit on the number of atoms of this element that may appear in the library entry. If an element appears only in the **Max** field, there is no lower limit on the number of atoms of this element that may appear in the library entry.

Include Other Elements If selected, other elements may be present in the library entry. If not selected, the library entry must contain only the elements specified in the **Min** and **Max** fields.

Flags Specifies a range of values within which a library entry **Flags** parameter must lie in order for the entry to appear in the Hits List. The **Flags** parameter is only relevant to user libraries.

User flags These are strings of one or more characters that have been entered in the user library. Enter the required text in the **User flags** field.
The search for the **User flags** text is always case sensitive. If **Apply exact** is not selected, the library entry must contain the characters specified in the **User flags** field. These characters can appear in any order in the matching library entry.

Apply Exact If selected, the library entry needs to contain the characters specified in the **User flags** field in the exact order in which they are entered.
For example, if the **Flags** parameter is set to Bv, BpKv, vKpB and KBvp will pass a nonexact search; only KBvp will pass an exact search.

User Values These parameters specify a range within which a library entry User Value must fall in order for the entry to appear in the Hits List. The **User Values** parameter is only relevant to user libraries.

No. 1 and These are numeric values that have been entered in the user

No. 2 library. Select the **No. 1** and **No. 2** values as required.

Min and **Max** Enter a maximum and minimum value for each **User Value** in the **Min** and **Max** fields. To specify a particular **User Value**, make the **Min** and **Max** values equal.

3. Click **OK**.

Starting a Library Search

You can initiate a library search from either Library or Spectrum.

➢ Click  from the Library toolbar

OR

Select **Search** from the Library **Process** menu.

OR

Click  from the Spectrum toolbar, or select **Library Search** from the Spectrum **Tools** menu.

Library Search Results

The result of a library search is a list of library compounds, or hits, whose spectra give the best match with the unknown spectrum.

The results are displayed in four windows:

Hit List — Gives a text listing of the best hits. The Hit List can be formatted to display a variety of information about each hit including compound name, fit values, formula, and molecular weight.

Hits — Shows the unknown spectrum followed by the spectra of the best hits.

Structure — Shows the chemical structure of the currently selected hit.

Delta — Shows the difference between the unknown spectrum and the spectrum of the current hit.

The mass spectral library is stored in the Idendb sub-directory in the TurboMass installation directory. The mass spectral structures library is stored in the Structdb sub-directory in the TurboMass installation directory.

Automatic Library Search

The library search application used for identifying spectra by matching them with a standard library (for example, NIST) works on a single spectrum when started from the Spectrum display. Chromatogram has an automated library search facility to automatically search a number of spectra in a chromatogram.

Note that while automatic library searching can work well for chromatographically well-resolved peaks, complex chromatograms will probably require manual background subtraction and library searching.

Using automatic library search in fully-automated mode

1. In the Chromatogram window, set the display range and integration threshold values to limit the integrated peaks to only those you wish to library search.

2. In the Chromatogram window, click  or select **Lib Search Peaks** from the **Process** menu.

3. The Library search process performs a search for the first peak in the list and displays the Print dialog.

4. To print results for all currently displayed Library windows, select **All Windows**.

5. To print results for the currently selected window, select **Current Window**, and click **OK**.

6. All other spectra matches will also be printed out in this format.

Using automatic library search in semi-automated mode

1. In the Chromatogram window, set the display range and integration threshold values to limit the integrated peaks to only those you wish to library search.

2. Integrate the chromatogram of interest.

3. To append specific peaks, select **Peak List Write** from the Chromatogram **Edit** menu, select the desired peaks, and click **Append**. Repeat for each peak required.

   OR

   To append all peaks, click **Append All**.

4. To automatically remove calculated background spectra, select **Auto Refine** from the Library Hits **Process** menu.

5. Select **Search Peak List** from the Library Hits **Process** menu.

   The Library search process performs a search for the first peak in the list and displays the Print dialog.

6. To print results for all currently displayed Library windows, select **All Windows**.

   OR

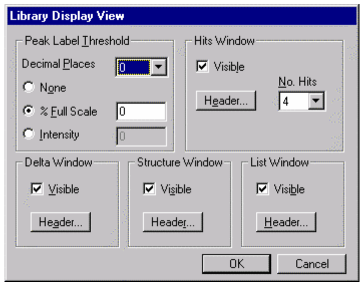
   To print results for the currently selected window, select **Current Window** and click **OK**.

   All other spectra matches will also be printed out in this format.

Manipulating the Library Display

The appearance of the display can be changed from the Library **Display** menu.

1. Select **View** from the Library **Display** menu to open the Library Display View dialog.



2. To display a window, select **Visible** for that window.

3. Edit the Library Display View dialog parameters for each of the Library windows, and click **OK**.

Hits Window	Specify how many hits (1 to 4) to display with the search spectrum in the **No. Hits** drop-down list.
Header	Displays a header at the top of each window. Clicking **Header** opens the Header Editor, where you can edit the header information. For more information about using the Header Editor, see *The Header Editor* on page 54.

Peak Label Threshold

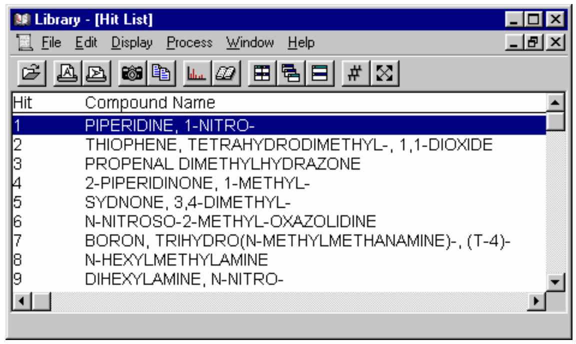
These parameters change peak labeling in the **Hits Window** and **Delta Window.**

Decimal Places	Select 0 to 4 from the **Decimal Places** drop-down list to specify the number of decimal places to which peaks are labeled. You can set a threshold for labeling peaks with mass.
None	If selected, TurboMass does not display mass labels for any peaks.
%Full Scale	If selected, this parameter sets a relative intensity threshold for peak labels.
Intensity	If selected, this parameter sets an absolute intensity

threshold for peak labels. Select **Intensity** and enter an intensity value.

4. Use the **Window** menu commands to arrange the different Library windows.

Hit List Window



The Hit List window gives a text listing of the best 20 hits resulting from the library search. These hits are listed in order of either reverse or forward fit, depending on which order was selected as the **Ranking** parameter in the Library Search Parameters dialog. You can format the Hit List window to include the following about each hit:

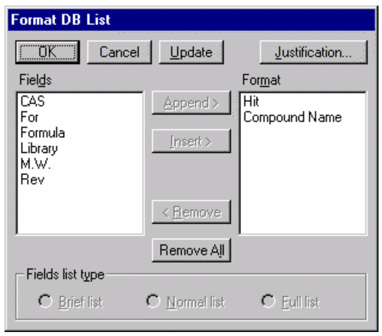
- Hit number.
- Compound name.
- Forward fit value.
- Reverse fit value.
- Chemical formula.
- Molecular weight.
- Library entry number.

- Library.
- CAS number.

The current hit is that selected in the Hit List window. It is the first hit that is displayed in the Hits, Delta, and Structure windows. You can make any other hit the current hit by selecting it in the Hit List window.

Modifying the fields displayed in the Hit List window

1. Select **Format List** from the Library **Edit** menu to open the Format DB List dialog.

   The **Format** list contains the fields currently displayed in the Hit List window. The **Fields** list contains additional fields available for display. To change which fields are displayed, edit these two lists.

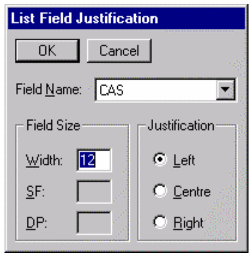
2. To add a field, select the field you want to add from the **Fields** list, and click **Append**.

3. To remove a displayed field from the Hit List window, select the field you want to remove from the **Format** list, and click **Remove**.

4. To insert a new field between two currently displayed fields, select the field you want to insert from the **Fields** list, then in the **Format** list select the field before which you want to insert the new field, and click **Insert**.

5. To modify the justification for any fields, select the field for which you want to change the justification from either the **Fields** or **Format** lists, click

Justification to open the List Field Justification dialog, select **Left**, **Right** or **Center** justification, modify the **Field Size Width**, Significant Figures (**SF**), and Decimal Places (**DP**) as required, repeat as required, and click **OK** to return to the Format DB List dialog.



6. Repeat steps 2 - 5 as required for each change you want to make to the Hit List window fields.

7. To view the results of your changes without exiting the dialog, click **Update**.

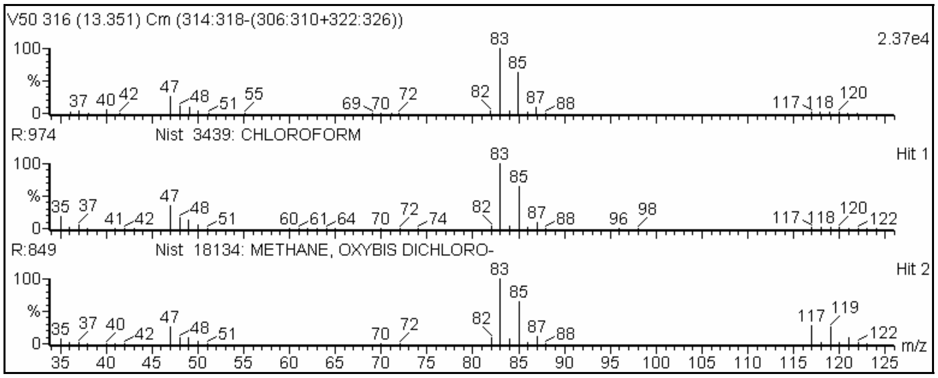
8. Click **OK**.

Hits Window

The Hits window displays the search spectrum with up to four of the hits spectra.

The header above each hit spectrum shows the hit number, fit value, the library name, library entry number, and the compound name.

The mass axis can be zoomed to expand a region of particular interest; these changes are also reflected in the Delta window.



You can manipulate the display in a number of different ways:

- Determine which hits are displayed.
- Change the range of the mass axis.
- Restore the display.

Determining which hits are displayed:

1. The first hit displayed is always the current hit, which is the hit selected in the Hit List window.

2. To change the number of hits displayed, select **View** from the Library **Display** menu, and change the **No. Hits** value.

   The Hits window displays up to four of the next best hits.

Changing the range of the mass axis (zoom):

➢ Left-click at one end of the region of interest and move the mouse horizontally to the other end.

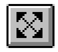
   TurboMass indicates the range you have selected. Do not go beyond the bounds of the axis. When you release the mouse button, TurboMass redisplays the selected range to fill the current window.

   OR

1. Select **Range From** from the Library **Display** menu.

2. Enter new mass axis **From** and **To** values, and click **OK**.

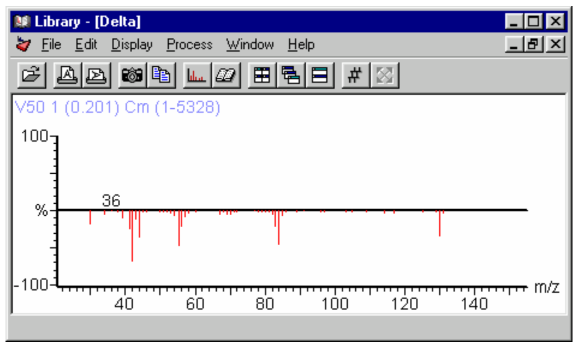
Restoring the displayed mass axis range:

➢ Toggle the  tool button to restore the display to its previous mass range or to the default mass range.

OR

Select **Range Default** from the Library **Display** menu to display the default mass range.

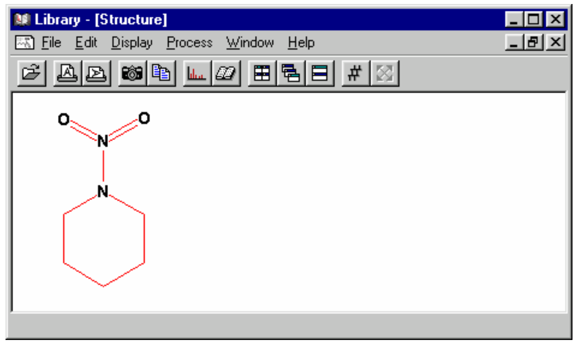
Delta Window



The Delta window shows the difference between the search spectrum and the currently selected hit. Positive peaks are those that are more intense in the search spectrum than in the hit spectrum. Negative peaks are those that are more intense in the hit spectrum than in the search spectrum.

The 100 % annotation point of the intensity axis refers to the base peak intensity of the spectra, before subtraction. The mass axis of the Delta window is always the same as that of the Hits window and cannot be changed independently.

Structure Window



The Structure window shows a graphical representation of the chemical structure of the currently selected hit.

The structural pictures are derived from structure data supplied by the United States National Institute for Standards and Technology (NIST) and are their copyright. Not all NIST Library entries have associated structures. If the currently selected hit has no associated structure, the message "No structure found" appears in the Structure window.

If the Structure window is blank, it may be because it is too small to contain the structure. As a quick check, try maximizing the window.

Structures are associated with library entries by their CAS number. If you create a user library and enter the correct CAS numbers, you can view the structures for the entries.

The mass spectral structures library is stored in the Structdb sub-directory in the TurboMass installation directory.

Printing the Results of a Library Search

You can print the library search results displayed in currently selected Library window.

Printing the library search results

➢ Click  or  to print in portrait or landscape format, respectively.

OR

Select **Print** from the Library **File** menu.

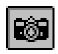
You can choose whether to print all windows or only the current window.

Copying To and From the Windows Clipboard

The Windows clipboard can temporarily store information that is being transferred from one application to another. You can use the Clipboard to move data out of a window as a picture and in some cases as a text list.

Copying a picture to the Clipboard

1. Set up the picture you want to copy in its window, and select the window.

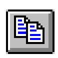
2. Click 

   OR

   Select **Copy Bitmap** from the **Edit** menu.

   The displayed picture is transferred as a bitmap to the Windows clipboard.

Copying the current hit list to the Clipboard

➢ Click  to copy the current hit list to the Clipboard.

Retrieving data from the Clipboard

Many Windows applications have an Edit Paste or similar command to read data in from the Clipboard. Consult the documentation for more information.

You can use the Edit Paste command to copy bitmaps into the Spectrum and Chromatogram applications.

Refining the Search Spectrum

The Refine process is used to identify only those masses that contribute to a specific peak in the TIC. In this way, Refine Search removes small peaks that are the result of background noise, and can therefore improve library search results. You supply two parameters for the Refine process: Window Size and Noise Threshold.

The refine algorithm generates the summed mass chromatogram over a range of 1 Da centered on each integer mass, in turn. It examines these chromatograms for a number of scans equal to the window size around the peak top scan. If a peak is present in this range for which the topmost point is within one scan of the peak top scan, and more intense than the noise threshold value, then this mass appears in the refined spectrum.

To refine the search spectrum

1. Specify new Refine parameters by choosing Refine from the Library Process menu to open the Refine Spectrum dialog.

Enter values for Window Size and Noise Threshold. Window Size is the half-width in number of scans at the baseline of the TIC peak of interest. For the first run, set Noise Threshold to zero to show all peaks, and choose OK.

If the noise level in the refined spectrum is unacceptable, repeat the Refine operation with a higher Noise threshold setting. Values in the 0-10 range are recommended.

OR

- Refine the current spectrum using the current Refine parameters by choosing  from the Library toolbar.

Auto Refine

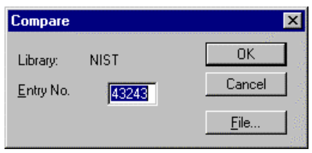
- To automatically use the refine parameters in all searches, select Auto Refine from the library Process menu. A check mark appears next to the item if it is selected. To turn this option off select it from the menu again. It is especially useful with automatic library searching from Chromatogram.

Using the Library Compare Process

The Compare process allows you to compare the search spectrum to a particular library entry. This can be useful if you have an idea of what the compound is or what type of compound it is, particularly if the compound in question does not appear in the top 20 hit list.

Comparing the search spectrum to a library entry

1. Select Compare from the Library Process menu.



2. Enter the number of the entry to which you want to compare the search spectrum. You can access a different library by clicking **File**, and click **OK**.

   TurboMass updates the Library display to show the results of the comparison in the Hit List, Hits, Delta, and Structure windows, if these windows are currently displayed. The format of the display is the same as for a normal search except, of course, there is only one hit.

Using the Library Subtract Process

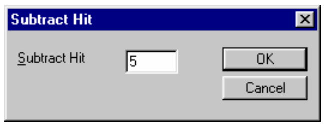
The Subtract process allows you to subtract the spectrum of a particular hit from the search spectrum. The resulting subtracted spectrum becomes the new search spectrum, and the library search can be repeated.

The Library Subtract process can be useful if you suspect that the search spectrum is a mixture of more than one compound. A mixture is indicated by a high Reverse Fit and low Forward Fit value. If you subtract the spectrum of one of the hits from the search spectrum and repeat the library search, the other component of the mixture now appears high on the Hit List. For mixtures that contain more than two compounds, this process can be used to identify compounds one at a time.

Subtracting a hit from the search spectrum

➢ Select **Subtract Hit** from the Library **Process** menu, enter the number of the hit you want to subtract, and click **OK**.

The subtracted spectrum becomes the new search spectrum.



Creating User Libraries

In addition to the libraries available from PerkinElmer, you can create your own "user" libraries that contain your own spectra. These spectra can come from raw data files or from existing libraries.

Creating a User Library

The steps involved in setting up a user library are as follows:

- Run the Spectrum application, and select the first spectrum that you want to add (append) to your library.
- Select **Library Append** from the Spectrum **Edit** menu.
- Click **File** and enter the name for the new library. Click **OK**. When prompted, click **Yes** to create the new library. Click **OK** to add the first spectrum.
- Using the TurboMass Spectrum application, select spectra one at a time to put into your library.
- For each selected spectrum, use the Library Append command from the Spectrum **Edit** menu to add to your library.
- In the Library application, select **Edit Library**, and set up the text data for each entry.
- Use the **Index Library** command from the Library **Process** menu to create the Presearch file for the new user library.

Once you have created a user library, you can add new spectra to it at any time by repeating these steps.

Creating a new user library

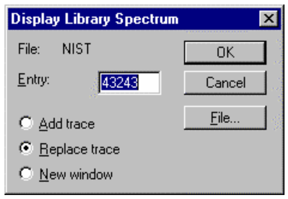
1. Open the Spectrum application.

2. Display the first spectrum you want to append to the library by doing one of the following:

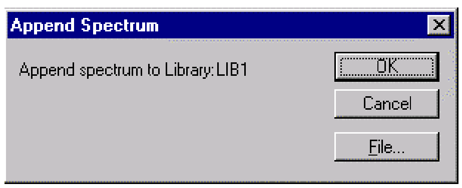
   To add spectra to an existing user library, display the spectrum you want to append to the library.

   OR

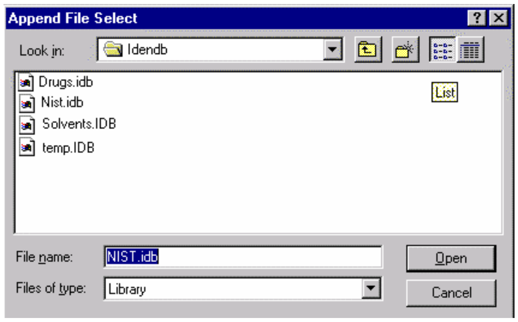
   To add spectra from a different library to an existing user library, display the library entry that you want to append to the new user library by selecting **Library Get Spectrum** from the Spectrum **Edit** menu, enter the number of the library entry you want to display, and click **OK**.



3. Select **Library Append** from the Spectrum **Edit** menu.
   The Append Spectrum dialog is displayed.



4. If the current library is the one you want, click **OK**. If not, click **File** to display the Append File Select dialog, enter or select the desired library file, and click **OK** to add the first spectrum into the new user library.



5. Enter a new file name for the user library, and click **Open**.

6. Click **OK** to add the first spectrum into the new user library.

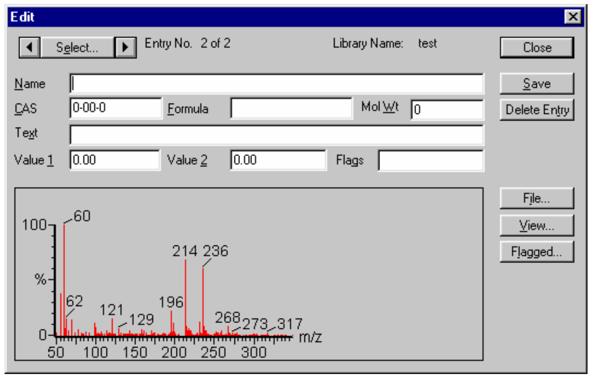
Adding Text Data to the Library Entries

Once you have appended a spectrum to a user library, you need to edit it to add text data such as Compound Name, Text, CAS Number, Formula, and Molecular Weight.

You can also add two numerical User Values and User Flags for the entry. These can be used to hold information about the compound. These fields can then be used as library search filters.

Entering text data for a user library entry

1. Select **Library** from the Library **Edit** menu to display the Edit dialog.



2. Select the entry that contains the data you want to enter or modify, and then enter the data.

Name The compound name for the entry up to a maximum of 128 characters.

CAS The Chemical Abstracts Sequence (CAS) number for the compound. The CAS number is used to link library entries to their chemical structures in the Structures Library for display in the Structures window. The CAS number has the format "x-yy-z", where:

x is a string of numbers; for example, 12398 or 6;

yy is a two-digit number string; for example, 23 or 07;

z is a one-digit number string; for example, 7 or 0.

Formula The elemental formula for the compound.

Elemental formulas are entered in "standard" format as an element symbol, followed immediately by its count if greater than one, and then immediately by another symbol, as relevant.

For example, consider Formula set to "C6H20NClBr2". Enter in the standard upper and lower case format. Note that, "Cl" does not need a "1" after it and that there are no spaces. The specific order of elements is irrelevant. **Formula** and **Mol Wt** are compared within an entry and you are warned if there is a

discrepancy.

Mol Wt The molecular weight of the compound that is entered as an integer, based on nominal masses for elements. For example, H is 1 and Cl is 35. **Formula** and **Mol Wt** are compared within an entry, and you are warned if there is a discrepancy.

Text Any text to a maximum of 30 characters.

Value Any positive or negative, integer (no decimal point) or decimal point value. These values can be used when setting filters for library searches or in the Process Locate dialog.

Flags A string of one or more characters representing user-specific information. You can enter any characters you like, including spaces to a maximum of eight characters. The order and case of the characters are significant.

These values can be used when setting Filters for library searches, in the Process Locate dialog or when selecting the **Flagged** Entries parameter in the Edit Library dialog.

3. Repeat step 2 as necessary.

   Each time you select a new entry you are prompted to save the changes you have made.

4. Click **Close**, and click **Yes** to save changes.

Indexing a User Library

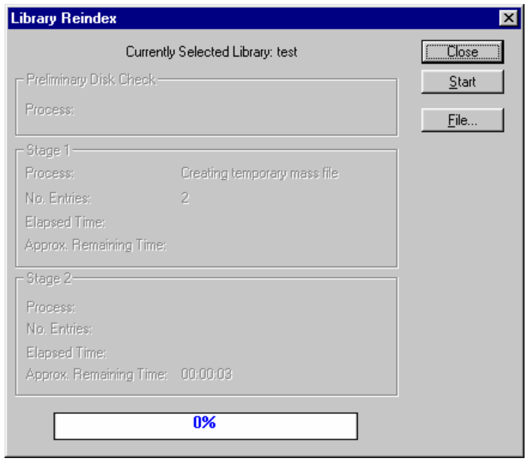
Before you can use a new or newly appended user library for searching, you must index the library to create a Presearch file for it. The Presearch file contains each library spectrum reduced to its eight most intense mass-weighted peaks.

Indexing a library requires a lot of processing and may take considerable time, depending on the size of the library. The Library Reindex dialog displays an estimate of the time required to index the library. Each time you add new entries to the library, you need to re-index it before you use it for searching.

Indexing a user library

1. Select **Index Library** from the Library **Process** menu.

   The Library Reindex dialog is displayed.



2. Click **Start** to begin the indexing process.

   A display keeps you updated on the indexing progress and gives you an indication of the remaining time required. When indexing starts, the **Start** button changes to the **Stop** button. You can cancel indexing at any time by clicking **Stop**.

3. When the indexing is complete, click **Close**.

Deleting Library Entries

You can only edit the text associated with a library entry; you cannot edit the spectrum itself. If you want to change the spectrum associated with a library entry, you must delete the entry and then create a new entry by appending the correct spectrum to the library.

Deleting a user library entry

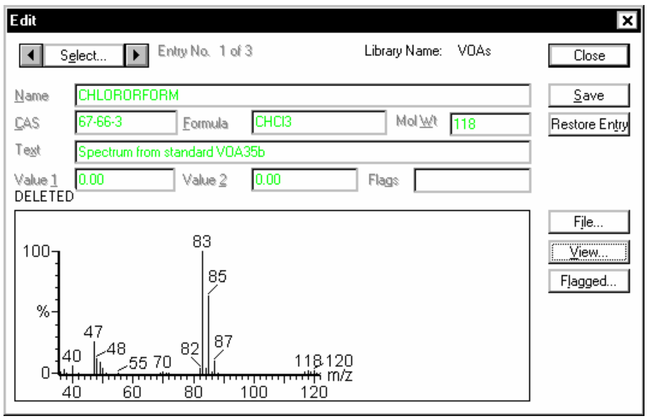
1. Select Library from the Library Edit menu to open the Edit dialog.

2. Select the entry to be deleted.

3. Click Delete Entry and confirm the deletion.

4. To view deleted entries, select View to open the View dialog .

   You see the text DELETED above the top left of the spectrum, and all input fields are unavailable. **Restore Entry** has replaced **Delete Entr**y and can be used to restore this entry. At this point, the entry has been **Flagged** as deleted but has not yet been physically removed from the library file.



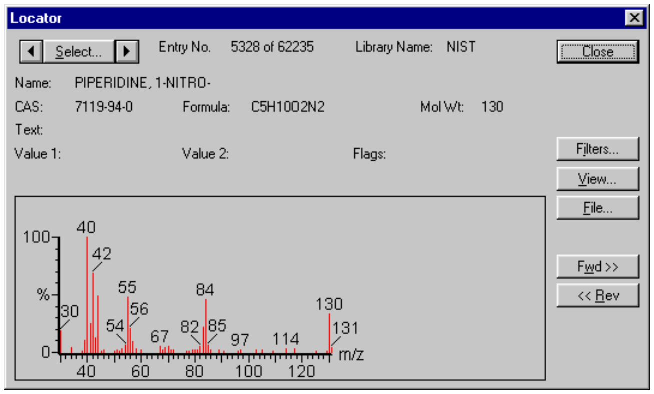
Using the Library Locator

The Library Locator can be used to look through a library. Filters can be set up and searches performed to select certain classes of compounds.

Locating one or more library entries

1. Select **Locate** from the Library **Process** menu.

   The Locator dialog is displayed.



   The Library Locator dialog contains the following information about a library entry: **Library Name**, **Entry No.**, Compound **Name**, **CAS** Number, **Formula**, Molecular Weight (**Mol Wt**), Spectrum and Structure. User Libraries may also contain Values 1 and 2, and User Flags.

   The Locator dialog can be used in two different ways: to select a particular entry for examination, or to set filter parameters that control the entries displayed by the Locate process.

2. Search the library:

   Manually: Use the scroll arrows to page through the library entries one at a time, or click **Select**, enter the desired **Entry No.** and click **Update**.

   OR

Using filters: Click **Filters** from the Locate dialog to set the match (locate) criteria, and click **OK** to confirm the criteria.

A message notifies you which filters are to be used for the Locate process.

TurboMass searches the library and displays the first entry that satisfies the locate criteria.

3. Click Fwd>> or <<Rev to find the next entry matching the locate criteria. Both operations start at the current entry and search in ascending (Fwd) or descending (Rev) entry-number order.

4. A message appears indicating the progress of the location. When the next suitable entry is found, TurboMass updates the display.

5. Repeat step 2 as required.

6. To stop the Locate process before it is finished, click Cancel.

7. When you have finished your search, click Close to return to the Library Hits window.

Map 17

Overview

The Map application provides a three-dimensional representation of an entire data file.

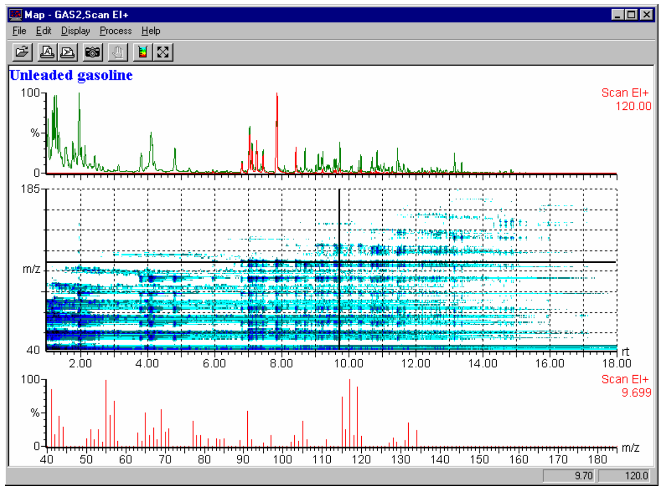


Figure 10 Map display of gasoline data file

The vertical axis displays mass/charge units (m/z) and the horizontal axis displays retention time in minutes. The third dimension is the intensity of a particular mass at a particular retention time, which is represented by a user selected color scheme.

The current cursor position is given by a pair of cross hairs. The mass chromatogram for the currently selected mass is displayed at the top of the Map window. The spectrum at the currently selected retention time is shown at the bottom of the Map window.

The Map program provides the ability to overview a complete data file very quickly. This is particularly useful for complicated GC/MS data files. The data file can be rapidly searched for particular masses, with the simultaneous display of mass chromatograms and spectra.

How to create a data file map

1. Select **Map** from the TurboMass top level **Process** menu

   OR

   Click .

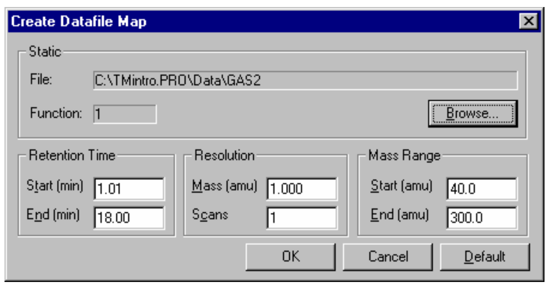
   The first time the Map program is loaded the Map window will initially be blank.

2. Click 

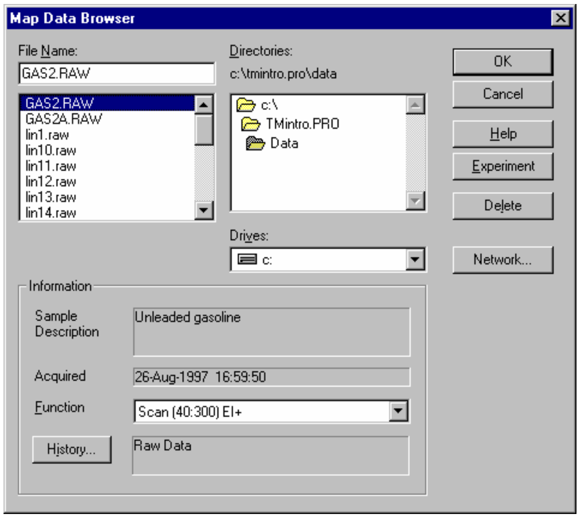
   OR

   Select **Open** from the Map **File** menu, or select **Create Map** from the Map **Process** menu.

   The Create Datafile Map dialog is displayed.



3. If you wish to change the data file select File to open the Map Data Browser dialog.



4. Select the new data file from the File Name list.

   You can access a data file on a different drive or directory.

5. Click OK to exit the Map Data Browser dialog.

6. Alter values as required in the Create Datafile Map dialog and click OK.

   A status bar at the bottom of the map window will keep you informed of the progress of the Map process.

Stopping the Map process before it has been completed

➢ Click 

OR

Select **Stop Process** from the Map **Process** menu.

About the Map Display

The Map display has three parts. The top trace shows a mass chromatogram of the currently selected mass. The lower trace shows the spectrum for the currently selected retention time.

The middle trace shows the map display of mass against retention time for the data file. Each block of color represents the intensity of a particular mass at a particular retention time. You can select a mapping mode and color scheme for the map display using the Display Scale options.

The currently selected mass and retention time can be changed by moving the cross-hairs cursor over the display. Moving the cursor in the vertical direction changes the current mass. Moving the cursor in the horizontal direction changes the current retention time. The current cursor position is shown on the right side of the status bar at the bottom of the display.

Double-clicking on the mass chromatogram will open the Chromatogram window with that mass chromatogram displayed. Double-clicking on the spectrum will open the Spectrum window showing that spectrum.

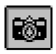
The Map Toolbar

The Map toolbar at the top of the Map window allows you to perform some commonly used actions by clicking a button.

 Selects a data file.

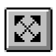
 Prints current window in portrait format.

 Prints current window in landscape format.

 Sends bitmap of current window to the Clipboard.

 Stops the current map process.

 Edits intensity scaling for map display.

 Toggles to restore the previous display range or to display the default display range.

You can toggle the toolbar display on/off by selecting **Toolbar** from the Map **Display** menu. When the toolbar display is selected, a check mark will appear next to it in the **Display** menu.

Selecting a Range to Map from the Data File

By default the Map program will create a map for the whole file, covering the full range of retention time and mass.

Reducing the mass and retention time ranges will require less memory and the map process will take less time. You may find this useful for large data files.

It is also possible to reduce the resolution used for the mass and retention time axes. Reducing the resolution will reduce memory requirements and may also enhance features in the data.

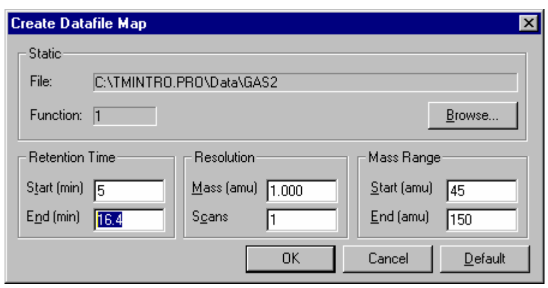
The Map program will sum all masses in a window equal to the mass resolution to create the map display. For example, if the mass range is set to 50 amu to 350 amu, and the mass resolution is set to 1 amu, a point will be plotted at 100 amu that is a sum of all masses between 99.5 and 100.5 amu.

The Map program will sum all scans in a window equal to the scan resolution to create the map display. Summing scans in the data file can also improve the signal to noise ratio, this will help to make peaks more visible and reduce the displayed noise.

Mapping part of the data file of interest

1. Select **Create Map** from the Map **Process** menu.

   The Create Datafile Map dialog is displayed.



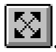
2. Enter values for the Mass Range and Retention Time range that you wish to map.

3. Click **OK**.

Manipulating the Display

You can alter the display, retention time, and mass axis ranges using the mouse or by using a menu command. The Map **Display** menu contains commands for changing the range of the mass axis and restoring the default display.

Altering the display range with the mouse

- Mass and retention time axes may both be expanded by clicking with the mouse on the spectrum. The previous state of the display can be restored by clicking .

Altering the range of the retention time axis

- Left-click at one end of the region of interest and drag the mouse horizontally to the other end. As you drag the mouse, TurboMass will indicate the range you have selected. Do not go beyond the bounds of the axis. When the mouse is released, the selected range will be redisplayed.

  This operation can be repeated as often as required.

Altering the range of the mass axis

- Left-click at one end of the region of interest and drag the mouse vertically to the other end. As you drag the mouse, TurboMass will indicate the range you have selected. Do not go beyond the bounds of the axis. When the mouse is released, the selected range will be redisplayed.

  This operation can be repeated as often as required.

Altering the range of both axes

- Left-click at one end of the region of interest and drag the mouse diagonally to the opposite. As you drag the mouse, TurboMass will indicate the range you have selected. Do not go beyond the bounds of the axis. When the mouse is released, the selected range will be redisplayed.

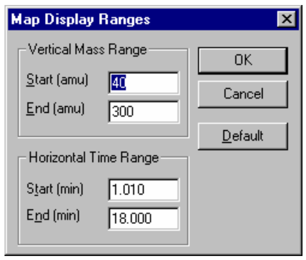
This operation can be repeated as often as required.

Restoring the display

➢ Clicking  toggles from restoring the display to its previous state to displaying the default range.

Altering the range of the mass axis from the Map menu

1. Select **Range** from the Map **Display** menu.



2. Enter new **Start** and **End** values for the mass and time axes as required.

3. Click **OK**.

Restoring the display to the default range

➢ Select **Default** from the Map **Display** menu.

Changing the Map Intensity Scaling

To enhance features within the data file it may be necessary to experiment with the map intensity scaling.

Each mass intensity is compared to the most intense mass in the data file range that is being mapped. Each mass is then mapped according to its comparative intensity to the corresponding color.

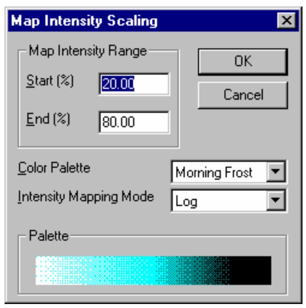
The value of **Start (%)** corresponds to the % intensity at which the color mapping starts, and the value of **End (%)** corresponds to the % intensity at which the color mapping ends. In the example, all masses with intensities less than 20 % on a logarithmic scale of the most intense mass would be shown in the first user color. All masses with intensities greater than 80 % on a logarithmic scale of the most intense mass would be shown in the last user color. All masses with intermediate intensities would be mapped to the other user colors.

Changing the map intensity scaling

1. Click 

   OR

   Select **Scale** from the Map **Display** menu.



2. Set the Intensity Mapping Mode.

   The options available are **Linear**, **Square Root** and **Log**. The log and square root intensity modes will give more weighting to lower intensity masses.

3. Set the Color Palette.

   The options available are White On Black, Black On White, Gray Scale, User or one of the Map color schemes. The Map color schemes available are Ocean Deep, Embers, Emerald Forest, Hot Metal, Cool Metal, Morning Frost, Polar Dawn and Tropical Lagoon.

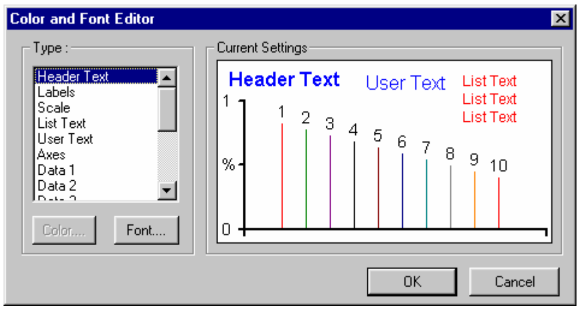
4. Define the User colors.

   The User colors are defined by selecting **Fonts and Colors** from the TurboMass top level **Customize** menu, and selecting the colors for Data 6 to 10.

5. Set the Map Intensity Range values, and click OK to create the map.

Changing user color scheme for Map display

1. Select **Fonts and Colors** from the **Customize** menu to open the Color and Font Editor dialog.



2. Select Data 6 to 10 in Type and change the colors as required.

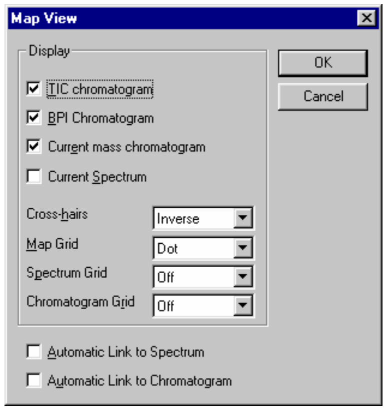
3. Click OK to update the Map display with the new colors.

Controlling the Appearance of the Display

The appearance of the Map display is controlled from the Map View dialog.

Changing the appearance of the Map display

1. Select View from the Map Display menu to open the Map View dialog.



2. Select the appropriate Map View parameters.

TIC chromatogram
If selected, the TIC chromatogram of the current data file is displayed at the top of the Map window. Deselect this checkbox to remove the TIC chromatogram.

BPI Chromatogram
If selected, the BPI chromatogram of the current data file is displayed at the top of the Map window. Deselect this checkbox to remove the BPI chromatogram.

Current mass chromatogram
If selected, the mass chromatogram of the currently selected mass is displayed at the top of the Map window. Deselect this checkbox to remove the mass chromatogram. All chromatograms displayed are overlaid on the same axes.

Current Spectrum
If selected, the spectrum at the currently selected retention time is displayed at the bottom of the Map window. Deselect to remove the spectrum.

Cross-hairs	This drop-down list controls the color used to display the cross-hairs cursor: **Inverse**, **Black**, **White** or **Axis color**. The cross-hairs cursor can be moved to change the currently selected mass and retention time.
Map, Spectrum, and Chromatogram Grid	Apply a grid to each part of the display. The grid pattern can be set to **Off**, **Dot**, **Dash** or **Solid** for each part of the display.
Automatic Link to Spectrum	If selected, the Spectrum window will be updated to show the current spectrum as the cross-hairs cursor is moved across the map display. Deselect to remove the link between Map and Spectrum.
Automatic Link to Chromatogram	If selected, the Chromatogram window will be updated to show the mass chromatogram of the currently selected mass as the cross-hairs cursor is moved across the map display. Deselect to remove the link between Map and Chromatogram.

3. Click OK.

Displaying the Chromatogram and Spectrum windows

- Double-click the mass chromatogram to display that mass chromatogram in the Chromatogram window.
- Double-click the spectrum to display that spectrum in the Spectrum window.

Displaying the Status Bar and Toolbar

The status bar at the bottom of the Map window displays:

- The current cursor position in terms of mass and retention time.
- The status of an ongoing process such as the Create Map process.

- The function of the currently selected menu item or toolbar button.

Displaying the status bar and toolbar

Toggle the status bar or toolbar display on/off by selecting **Status Bar** or **Toolbar** from the Map **Display** menu, respectively.

Selecting the Current Cursor Position

You can select the cursor position using the mouse or from the menu.

Changing the current cursor position

➢ Double-click the required position on the Map display.

  This position will become the current cursor position. The Spectrum and Chromatogram displays will be updated accordingly.

  If the cross-hairs cursor is displayed, you can change the current cursor position by left-clicking anywhere on the cross-hairs and dragging them to the new position.

  OR

  Select **Select Mass** or **Select Time** from the Map **Display** menu, enter the new value, and click **OK**.

Editing the Header Information

The Map Window has a customizable header. Various pieces of information such as raw data file name can be displayed here, as well as any user text. For more detailed information about the Header Editor, see *The Header Editor* on page 54.

Changing the displayed header

➢ Select **Header** from the Map **Display** menu, make the required changes, and click **OK**.

Printing from Map

To print the Map window:

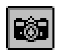
1. Select Print from the Map File menu.
2. Make any changes required to the print parameters.
3. Click OK.

Copying to the Windows Clipboard

The Windows Clipboard provides temporary storage for information that is being transferred between application programs (for example, word processors, spreadsheets, TurboMass). You can copy a bitmap of the Map window to the Clipboard and then, for example, paste the bitmap into a report written with a Windows compatible word processor.

Copying the Map display to the Clipboard

1. Produce the required display in the Map window.

2. Click 

   OR

   Select **Copy Bitmap** from the Map **Edit** menu to copy the contents of the window to the Clipboard.

3. To read the image into another application, select **Paste** from the other application's **Edit** menu.

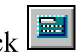
Molecular Mass Calculator 18

Calculating the Molecular Mass

The mass calculator can calculate two different molecular masses for a given chemical formula.

- **Monoisotopic mass:** Calculates the mass using the atomic weight of the most abundant isotope of each element.
- **Average mass:** Calculates the mass using the average atomic weight of each element taking into account the relative abundance of its isotopes.

Calculating the molecular mass for a given chemical formula

1. Select MW Calculator from the TurboMass Tools menu or click , to open the Molecular Mass Calculator dialog.
2. Enter the chemical formula using standard International Union of Pure and Applied Chemistry (IUPAC) notation.
3. To specify user defined elements or isotopes, follow the procedure Defining User Elements on page 546.
4. Select either Monoisotopic or Average Mass.

NOTE: *Monoisotopic mass is the usual choice for GC/MS.*

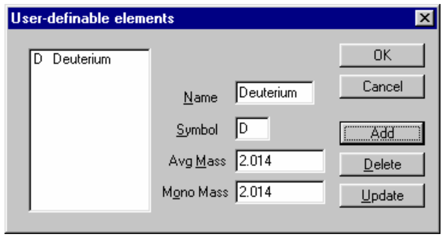
5. To display the calculated mass in the Mass field, click Calculate.
6. To edit the current formula and recalculate the mass, click Calculate.
7. To clear the current formula, click Reset.
8. To copy selected formulas or calculated masses to the Windows clipboard, click Copy.

   The Copy function is convenient for pasting ion masses into the SIR scan function.

Defining User Elements

You can define a user element by specifying its name, symbol, average, and monoisotopic masses.

1. In the Molecular Mass Calculator dialog, click **User element**s to display the User-definable elements dialog.



2. Enter the parameters and click Add to add the group to the list.

   You can add up to 10 elements, isotopes, or molecules to the list.

3. To edit a particular element or group, click Update.

4. To remove a selected group, click Delete.

5. Click OK to save the list and return to the Molecular Mass Calculator dialog.

6. Click Close to exit the Molecular Mass Calculator.

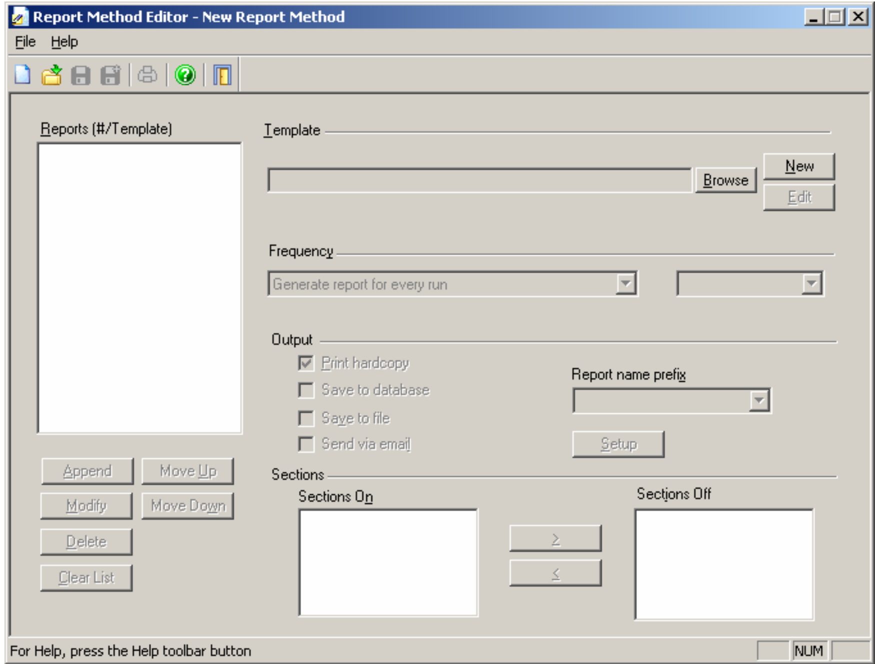
Report Method Editor 19

About the Report Method Editor

The Report Method Editor is an extension to the TurboMass software. It enables you to specify a collection of report definitions (Communiqué report templates and related parameters) that are printed sequentially. The Report Method is a dataset that you can specify in each row of the Sample List. It defines the reports to be generated following the analysis data or at the end of the Sample List. The Report Method will consist of a list of report templates and associated parameters, namely:

1. When the report will be generated (for all runs, for runs of a specific type, for only the last run in the sample list)
2. The output destination(s) of the report (print, save to database, save to file, send via email)
3. The printer (if printed) and/or the file name (if saved)
4. The email address(es) and message text (if emailed).
5. Sections of the report template to be printed or suppressed

NOTE: *Only a single report method can be loaded in the Editor at a time and only a single instance of the Report Method Editor can be run. If you edit a Report Method while the Editor is already open (e.g. by choosing the Open command from the context menu when the Report Method cell is selected in the sample table) then the new report method will replace the existing one, provided it is not in a modified state. If the current method is in a modified state the 'Do you want to save the changes to "<report method name>"?' warning dialog will be displayed.*



You open the **Report Method Editor** in one of two ways:

1. By choosing **Open** from the context menu when the Report Method cell is selected in the Sample List. If no method name is specified in the cell, or if there is currently no report method of that name in the **Project** directory, then the Report Method Editor will open in the 'New Method' state. If the cell contains the name of an existing report method then Report Method Editor will open in the 'Edit Method' state.

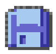
2. By choosing the **Report Method Editor** command from the TurboMass *Tools* menu. The default method will be the method most recently used. If there is currently no report method of that name in the project directory (that is the METHDB subdirectory in the project hierarchy), then the Report Method Editor will open in the 'New Method' state.

Report Method Editor Toolbar

The toolbar displayed at the top of the window lets you perform some common operations with a single click of the appropriate toolbar button. The default toolbar contains the buttons listed below. You can also customize the toolbar and add additional buttons for other operations.

 File New

 File Open

 File Save

 File Save As

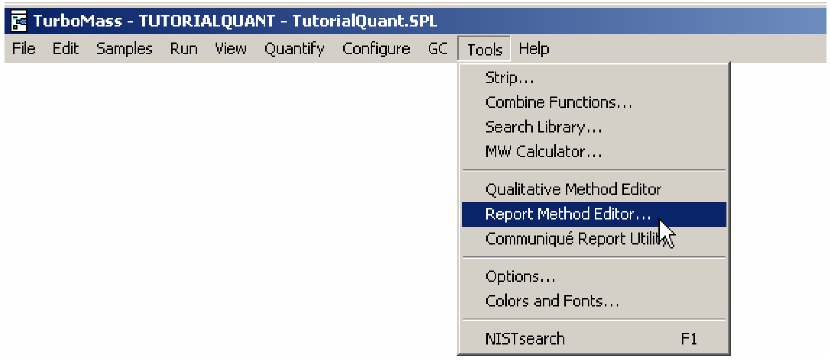
 File Print

 File Exit

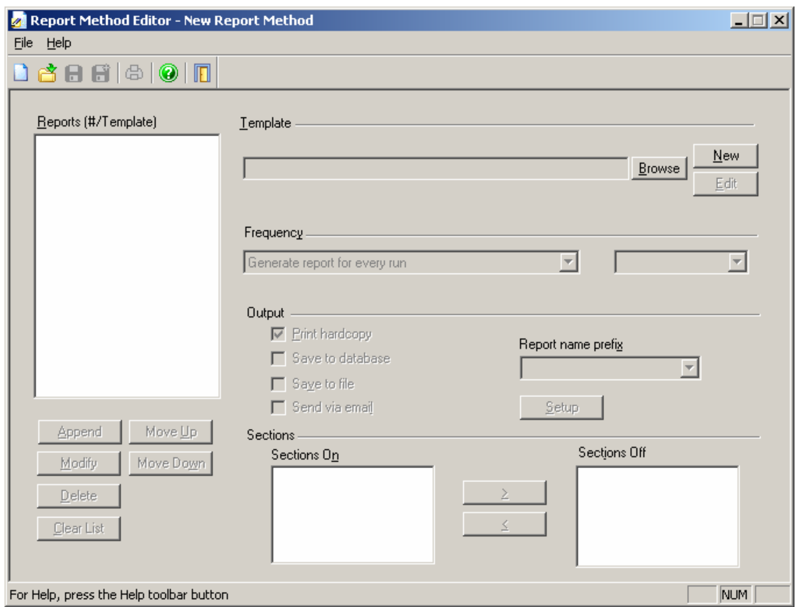
 Help Contents

Selecting an Existing Template

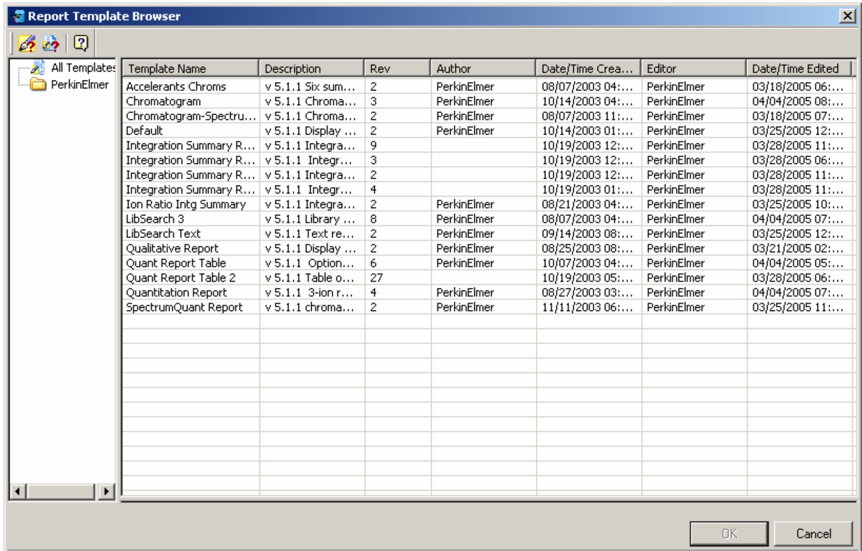
1. Select **Report Method Editor** from the *Tools* menu.



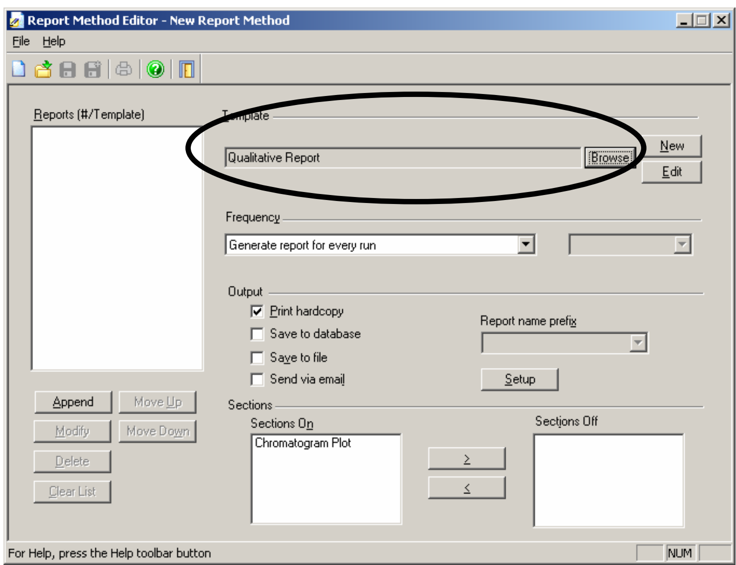
The Report Method Editor screen appears:



2. Click the **Browse** button to the right of the Template field. The Report Template Browser appears:



3. Select a Template name and click OK (for example, click Qualitative Report). This now appears in the Report Method Editor dialog:



4. Select the **Frequency** of reporting. The options available are:
   - **Generate report for every run**
   - **Generate report for every run of specified type**
     Selecting this option enables a second drop-down list. Here you select the type of run from the available options.
   - **Generate report only for final row in the sample list**

5. Select a desired Output type.

6. Click the Append button to add this template to the current method.

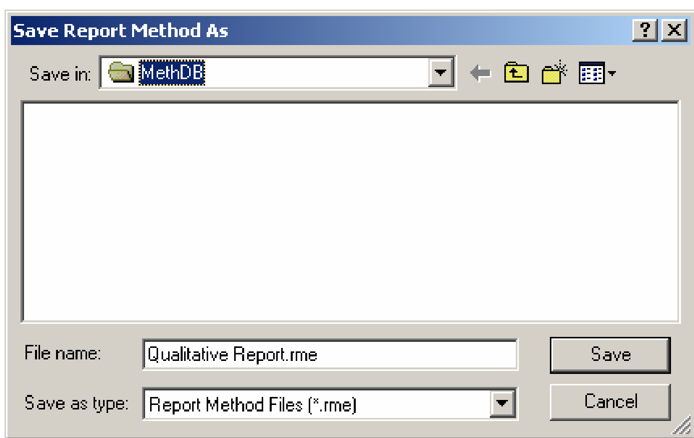
   This template appears in the **Report (#/Template)** field This is a display of the reports defined for the current method.

   When the list is empty (New Method, after **Clear List** or after all reports have been **Deleted)** the controls on the right will be set to default values. In this way the Append button is always enabled and valid.

   Using the **Move Up** and **Move Down** command buttons reorders the Reports in the list. Reports will be processed by report number (i.e. in the order in the list).

7. Select **Save As** from the Report Method Editor **File** menu.

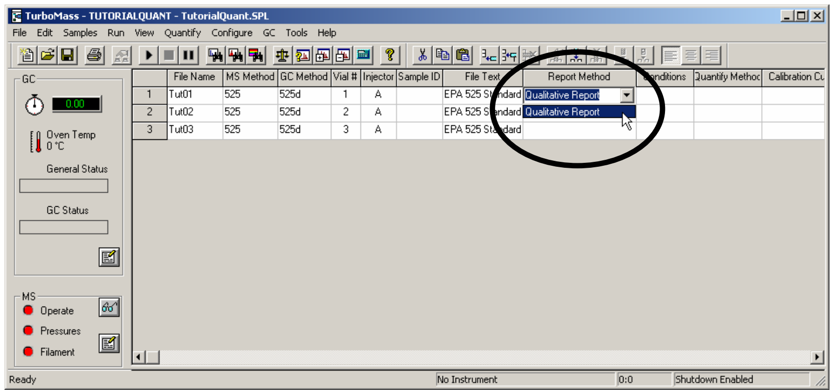
   The **Save Report Method As** dialog appears:



8. Type a File name for your Report Method (for example, Qualitative Report) then click **Save**.

   This Report Method is now available for the **Report Method** column of the **Sample List**.

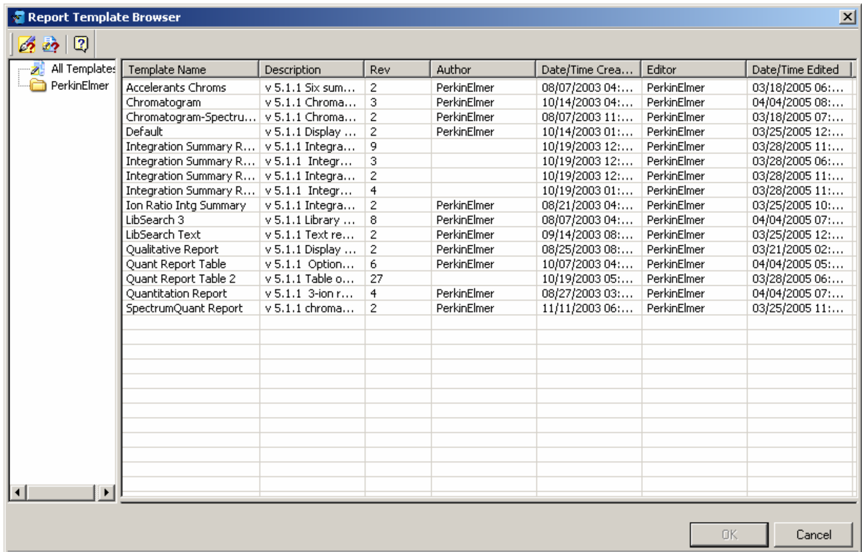
9. Double-click in the Report Method field and select Qualitative Method from the drop-down list.



10. Close the Report Method Editor by clicking the **Close** box (in the upper-right hand corner of the screen).

Report Template Browser

In the Report Method Editor dialog click the **Browse** button to the right of the Template field. The Report Template Browser appears:



➢ To locate a template in a large list:

Browse through the tree view on the left of the window to find your project folder.

or

1. Click the Define Template Filter button on the toolbar.
2. Set up the desired filter conditions in the Filter Templates dialog.
3. Apply the defined filter settings.

Filtering the Template List

The list of templates may become very large, thereby a filtering mechanism helps you locate the template of interest. The filter may be defined by accessing the report template filter dialog, using the toolbar button.

The setting of the apply template filter button determines whether or not the filter is active. This button can be in the 'up' or 'down' position. When the button is down the filter will be active and the list view will display only the templates matching the filter conditions.

Report Template Filter Toolbar

The toolbar displayed at the top of the Report Template Filter window contains the tool buttons listed below. The tool button functions are duplicated in the Report Template Filter menus.

	Displays the Template Filter dialog box.
	Toggles the defined filter for the template list on and off. The filter will be active when the button is in the 'down' position.
	Displays the Help window.

Communiqué Reporting 20

About the Report Method Editor

In this section we will show you how to use the Report Method Editor and Communiqué to modify an existing report template and create a new report template.

A vital aspect to the flexible reporting capabilities of the TurboMass software will be the data model. This defines the data that will be made available to Communiqué for design of the template and generation of the report. Most TurboMass data is available through the data model. This includes:

1. All existing quantitative data generated by the TurboMass Quantification process (including Area% and Norm% values).
2. The chromatograms and spectra defined by the Qualitative method and its processing.
3. Values associated with the multiple ion ratio identification process (ratios, pass/fail, etc.)
4. Peak plots associated with multiple ion ratio processing (for target compounds and internal standards).
5. Calibration curve plots associated with target compounds.
6. Library search spectral plot data and text results.
7. Quantification and Qualitative method parameters.

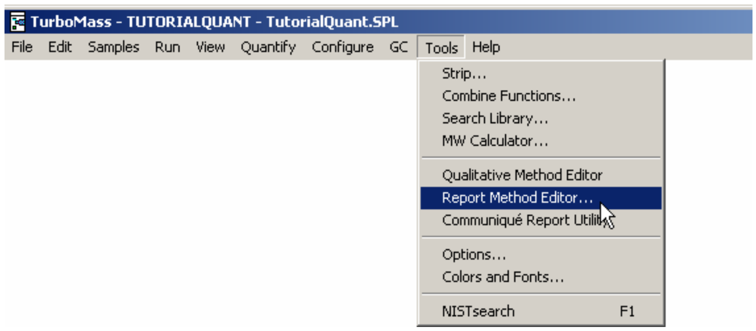
TurboMass creates a collection of Data Objects that appear in the Communiqué Report Creator.

In the **Communiqué Report Creator**, note that ***collections*** (in the Communiqué sense of the word) are indicated by parentheses '()' following the collection name for example Samples().

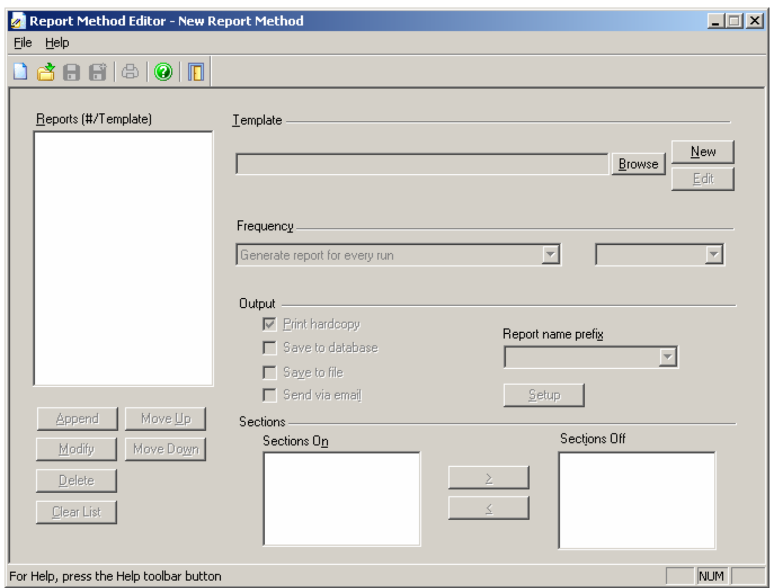
Opening a Report Template

To open an existing report template, follow this procedure:

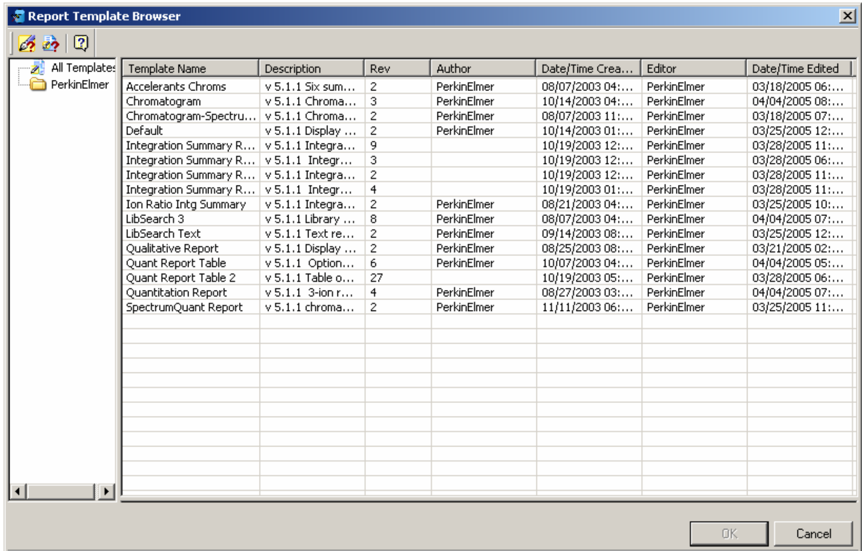
1. Select **Report Method Editor** from the *Tools* menu.



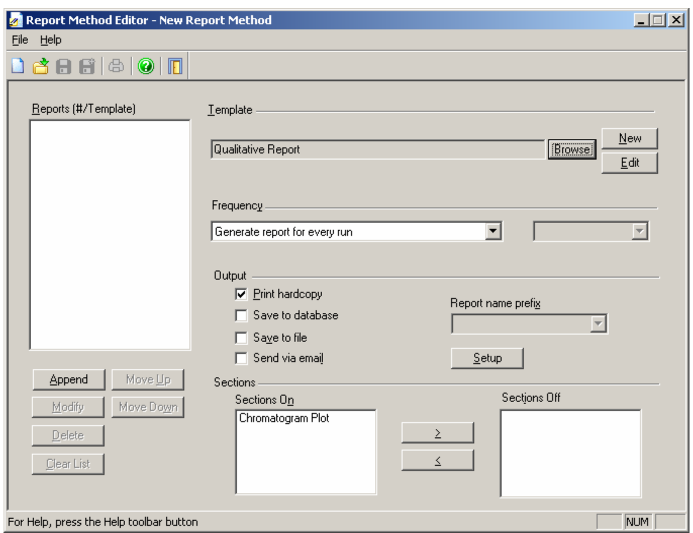
2. The Report Method Editor screen appears:



3. Click the **Browse** button to the right of the **Template** field. The Report Template Browser appears:

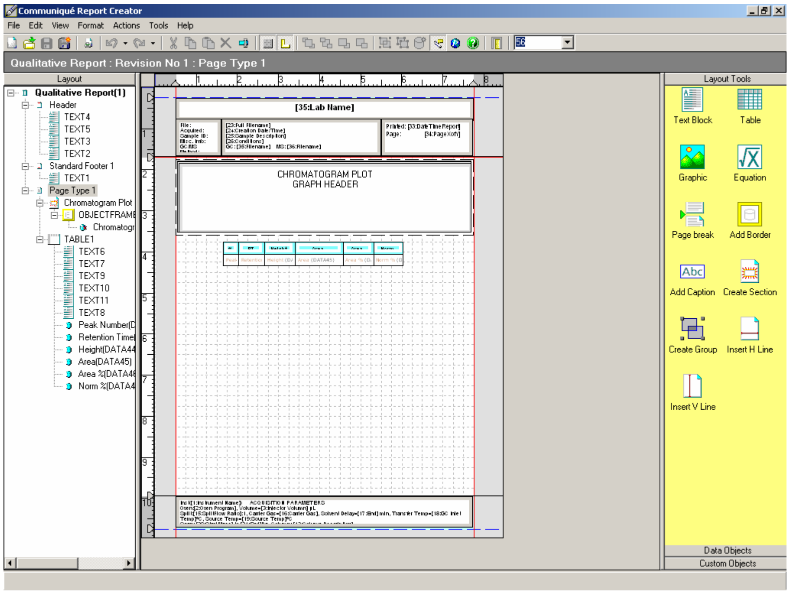


4. Select a template name and click **OK** (For example, click Qualitative Report). This now appears in the Report Method Editor dialog:



5. Click the **Edit** button.

   This launches the Communique Report Creator.

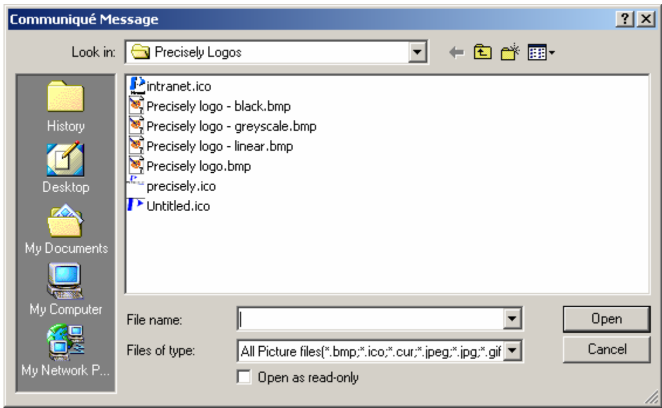


Modifying the Template

To modify the template, follow this procedure:

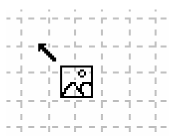
1. Add a graphic by clicking **Graphic** in the **Layout Tools** toolbox.

   A dialog similar to the following appears:



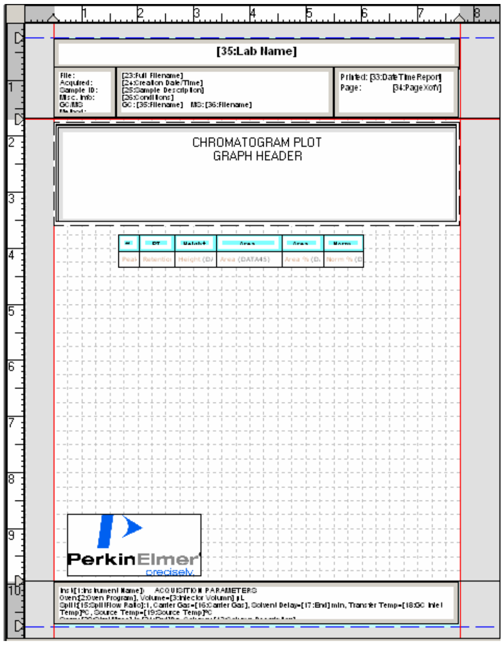
2. Browse to the directory where the graphic is stored and select it by clicking on it.

3. Move your cursor to the design page and click. The cursor changes to the following cursor:



4. Move your cursor to a desired spot on the page. Click the left mouse button, drag the mouse to scale the graphic to a desired size, then release the mouse button.

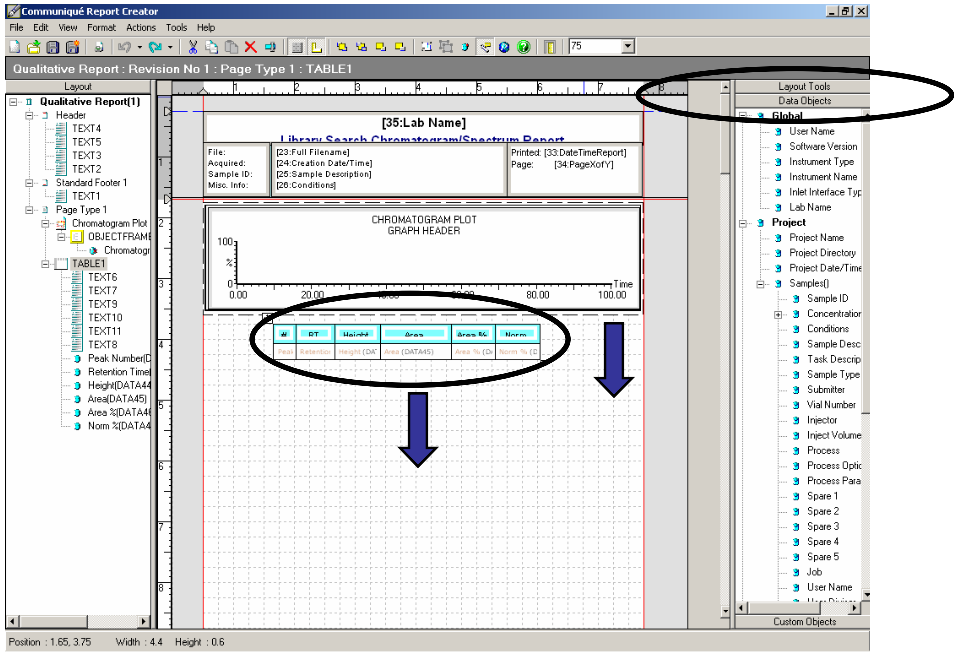
   The graphic appears on the page.



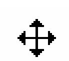
Adding a Data Object to the Template

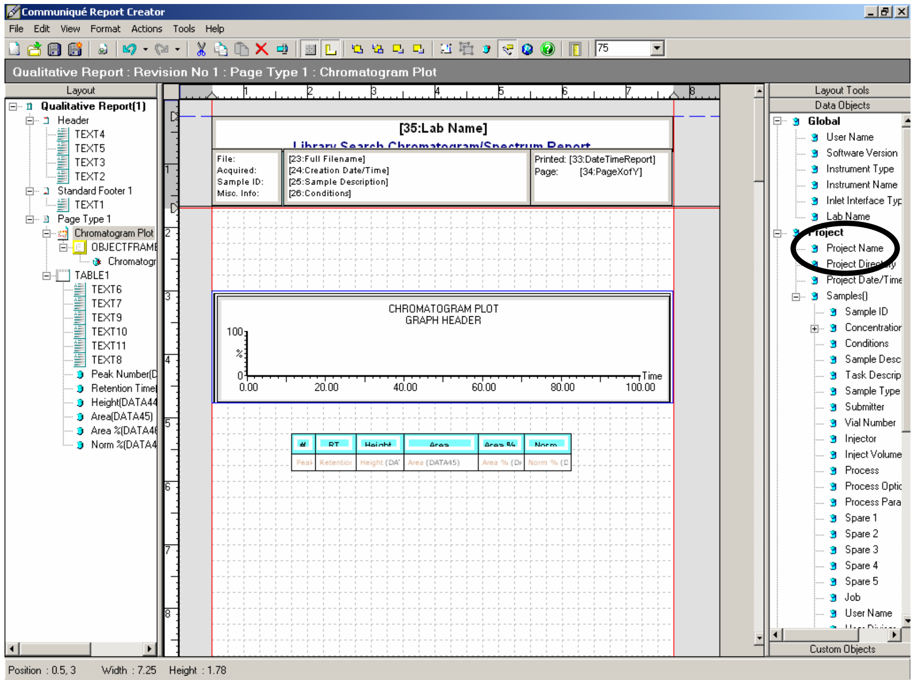
To add a data object to the template, follow this procedure:

1. Click on **Data Objects** to display the available data objects.



2. Move the *table* (see above) and then the *Chromatogram Plot* down the page to make room at the top of the Chromatogram Plot.

- To move the table and Chromatogram Plot, move your cursor over the table.
- It turns into  Now hold the left mouse button down and move your mouse to move the table.
- Next move the Chromatogram Plot the same way.

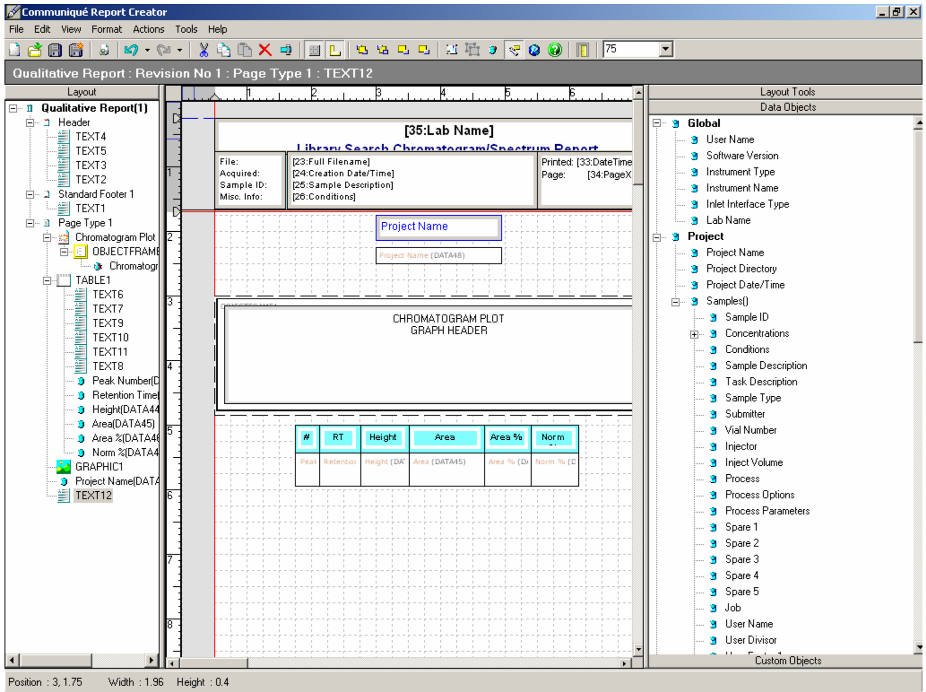


3. Click on **Project Name**, move your cursor to the designer page, the click where you want the Project Name to appear and drag it to the desired size.

4. Click on **Layout Tools** to display the Layout Tool selections, click on **Text Block**, move your cursor to a position on the designer page, click and drag to put the text block on the page. Position the cursor on an edge of the **Text Block** and hold the left mouse button down and drag the edge to the proper size.

5. Click in the **Text Block** and type (for example, Project Name).

6. Highlight the text and right click to display the text formatting options.



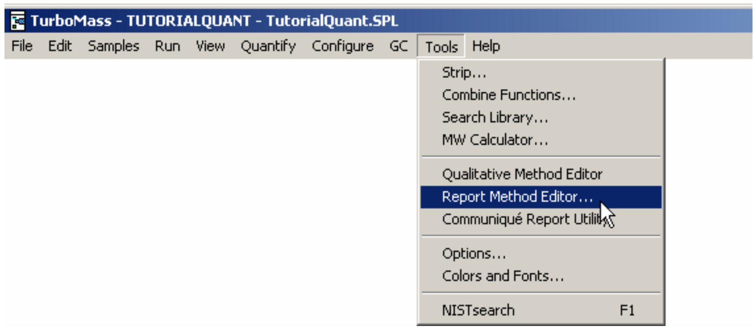
7. Click **Save As** from the *File* menu, name and save your file.

8. Exit the Report Designer.

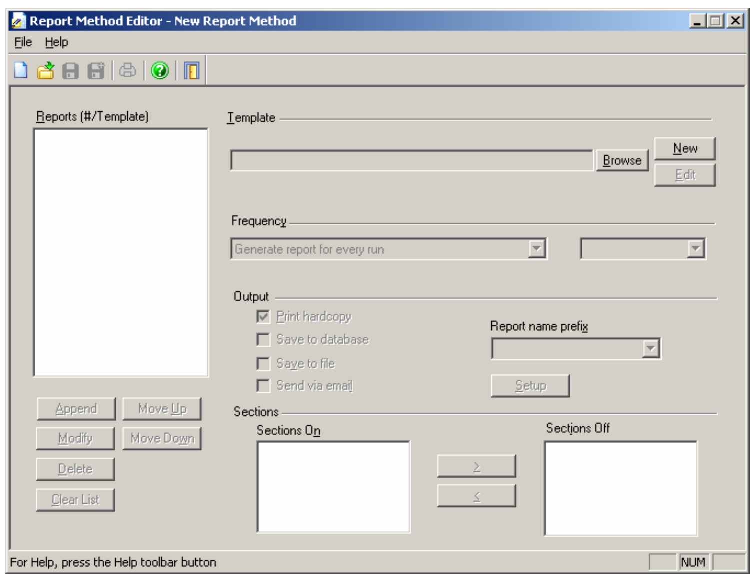
Creating a New Report Template

To create a new report template:

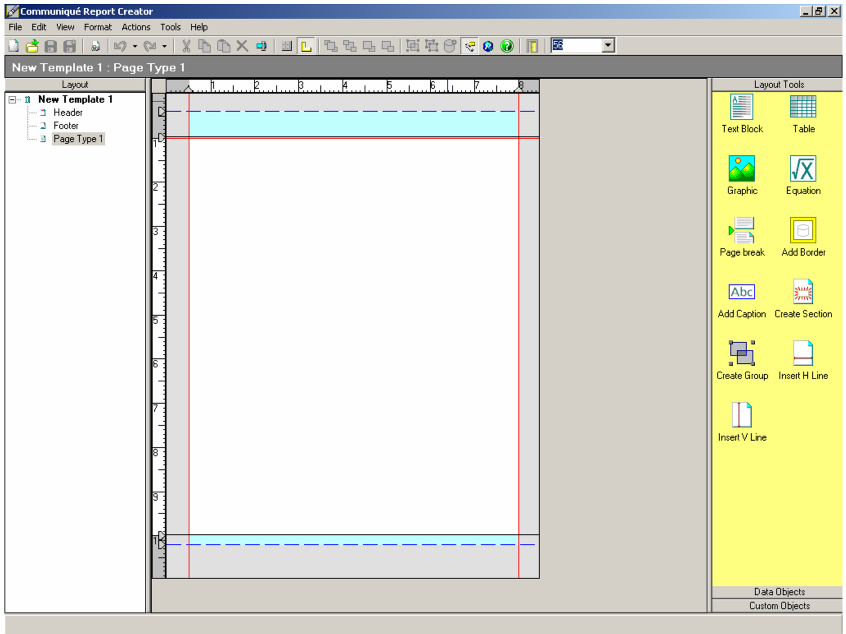
1. Select Report Method Editor from the Tools menu.



2. The Report Method Editor screen appears:

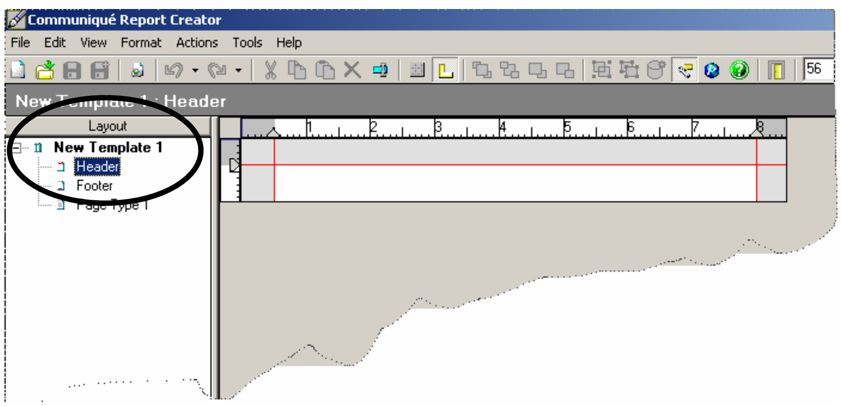


3. Click the New button to the right of the Template field. The Communiqué *Report Creator* appears:

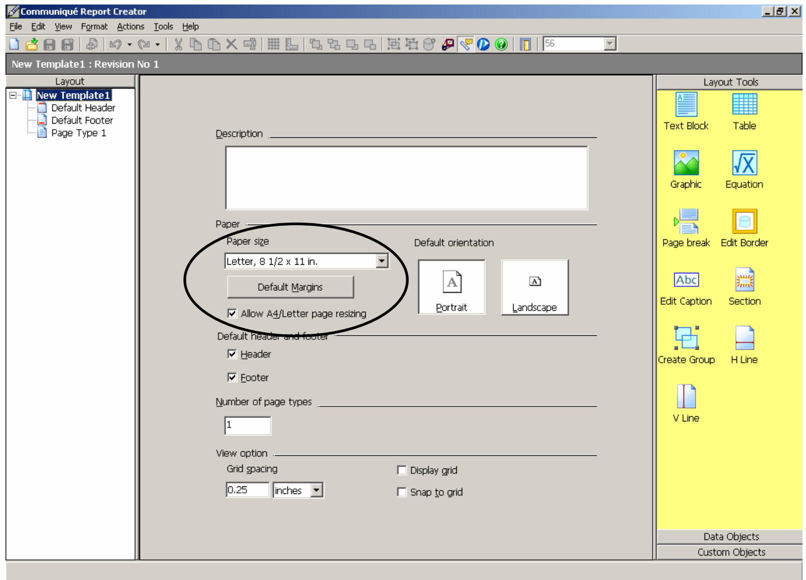


Add a Header and Footer

1. Click on Header in the Layout toolbox on the left of your screen.
   The Header appears.



If you click on New Template the template description page will be displayed. Here you can allow for A4/Letter resizing of your template. To properly use the non-A4 templates as the only set, the **Allow A4/Letter page resizing** option in each template's description page should be selected and in all cases the Paper drop-down list on the template description page should always be set to Letter so that the page size appears properly in the template editor.



2. Drag a **Text Block** into the Header. Label it "Qualitative Report Test1." Then format the text as follows:

   a. Highlight text and right-click to select **Format**.

   b. Select **Font** tab.

   c. Set to **Blue, 20 pt. Ariel, Bold**.

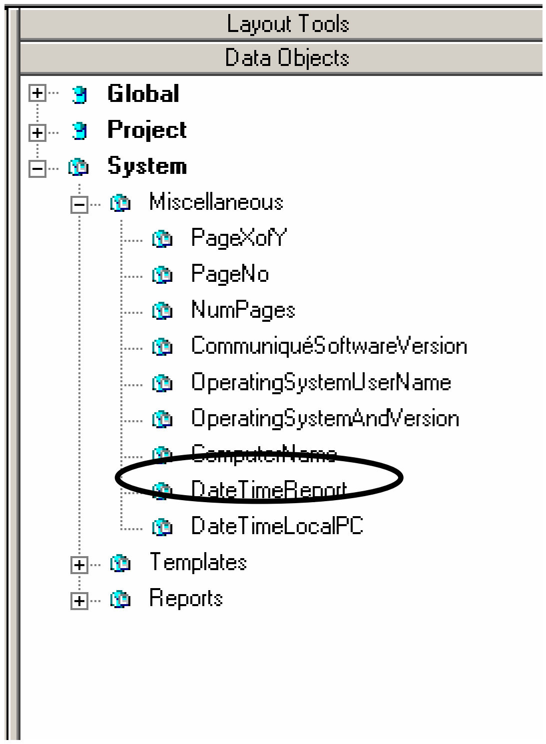
   d. Set **Paragraph** tab, alignment **Horizontal / Center**.

   e. Click **OK**.

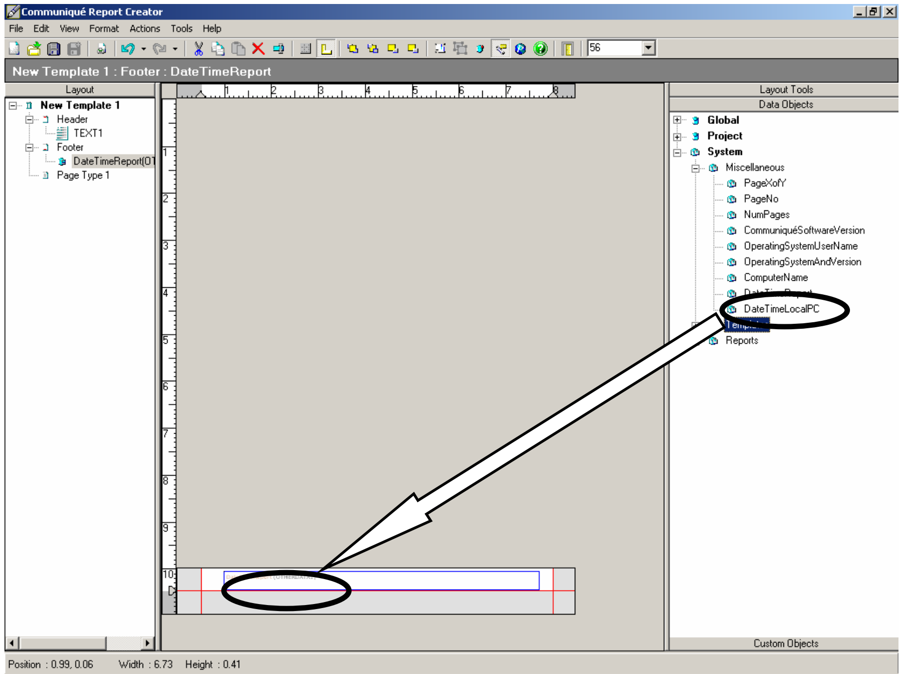
   f. Resize the **Text Block** so that you can see the text.

3. Click on Footer in the Layout toolbox on the left of your screen. The footer appears.

4. From the **Data Objects** toolbox, left click **DateTimeReport**.



5. Click in the footer, then size **Date Time Report** into the Footer to full width.



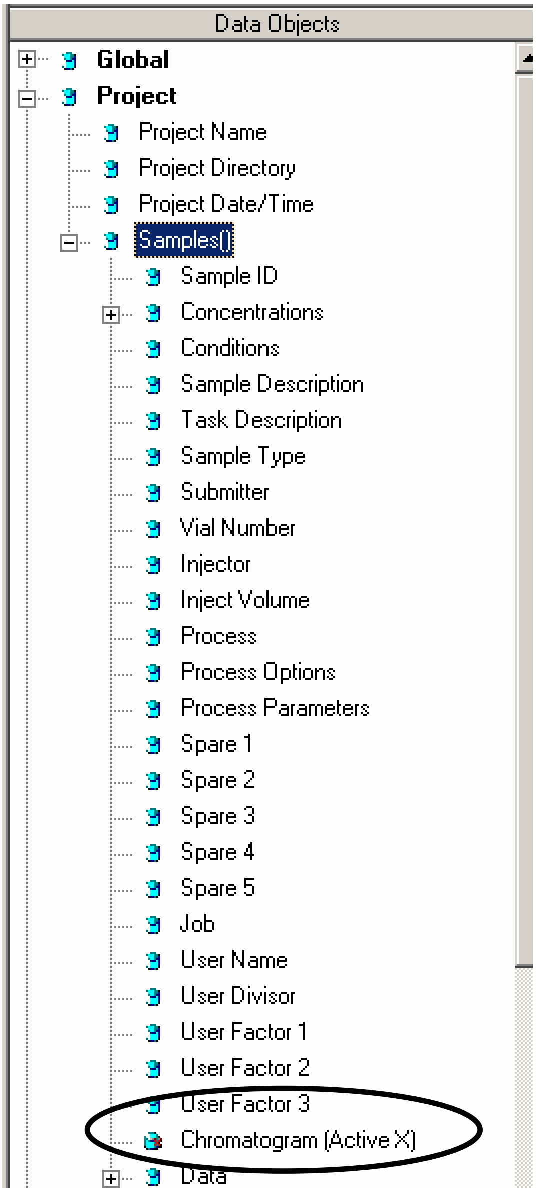
6. Click on **Page Type 1** in the **Layout** toolbox on the left of the screen. This will display the main body of the template.

Add Data Objects

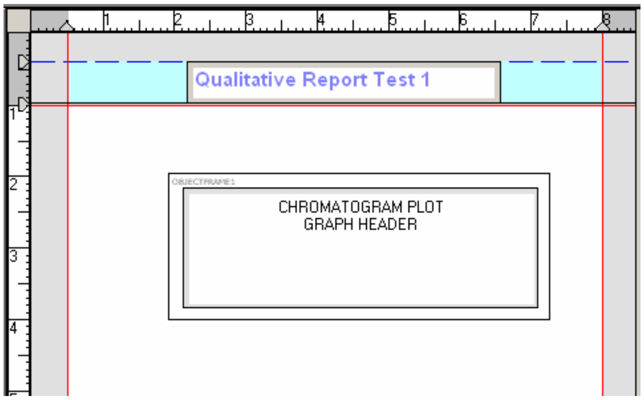
NOTE: *The Communiqué user interface supports click and drop rather than drag and drop. Simply left click on the object in the Data Objects tree and release the mouse button. Next, position the mouse pointer in the template, click and drag the pointer, then release. Use this same functionality for placing any object onto a template.*

NOTE: *To ensure that a CSV file puts data items on the same line, enclose all items that are required to appear on one line of the CSV file in a Communiqué Section object. All items enclosed in the Section should have the 'Down from Top' property set to zero (0). Also, all items should have the same 'Height' value set as the Section* itself.

1. Click on Chromatogram (Active X) in the Project > Samples() directory of the **Data Objects** toolbox (Graphic Data Objects have a small red "x" as their icon.



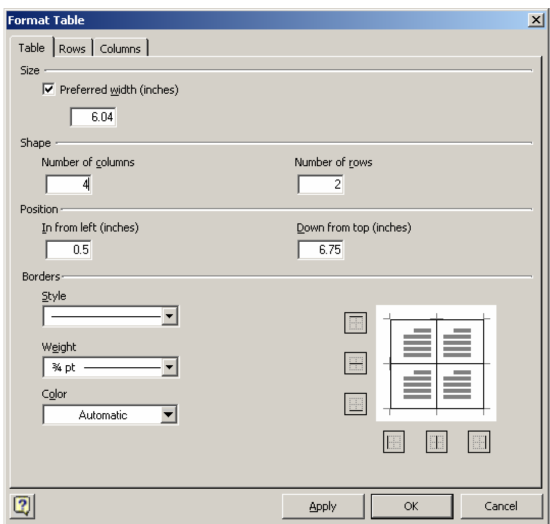
2. Left-click on Chromatogram (ActiveX), move the cursor to the center of the design page, then left click and hold the mouse as you drag the mouse to expand the box. The box displays as **CHROMATOGRAM PLOT GRAPH HEADER**.



3. From **Layout Tools**, left click on **Table** then move your cursor to the page and left click. A four column by two row table appears.

4. Select the table. Right-click Format.

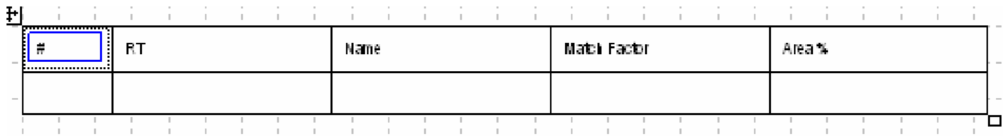
   The Format Table dialog appears:



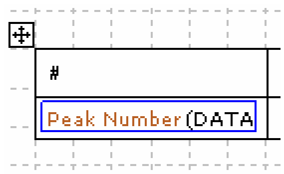
5. Change the Number of columns from **4** to **5** then click **OK**. If necessary, click on the **Columns** tab and change the Column width to 0.5.

6. Add text blocks to the top row of the table. Label each cell as follows; **#, RT, Name, Match Factor, and Area%.**

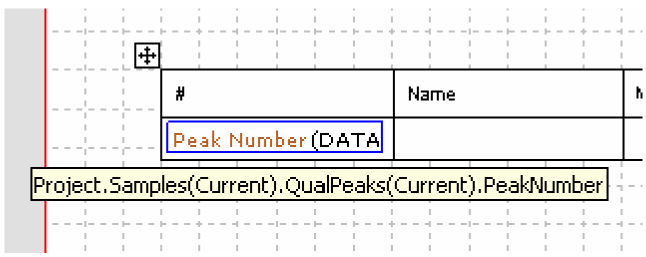
NOTE: *Remember to first put a Text Block (from the Layout Tools) in the table so that you can enter a label.*



7. Under "#" put Peak Number, from the Project / Samples() / Qualitative Peaks () path in the **Data Objects** toolbox.



If you move your cursor over **Peak Number (DATA)** the following appears:



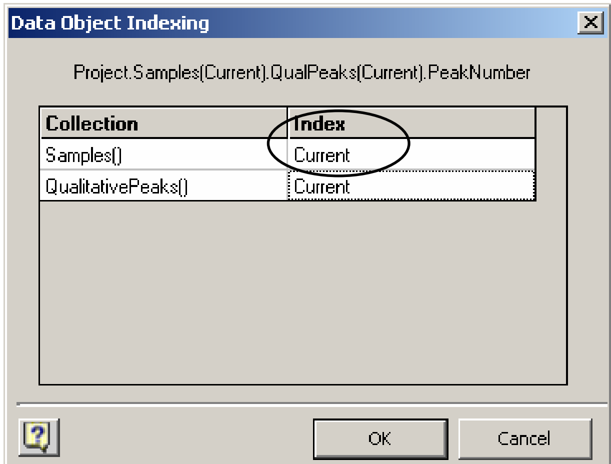
This information **Project.Samples(Current).QualPeaks(Current).PeakNumber** is the source string of the data. In this example, it will report the peak number of the current QualPeak in the current Sample.

About Samples; Current versus Last: The template is used to pull information from the data source during report creation. From the point of view of the data source, the most recent data (e.g., the current line on the Sample

List) is the last data entered into the data source. Therefore, to view data from the current line of the Sample List, use **Samples(Last)**.

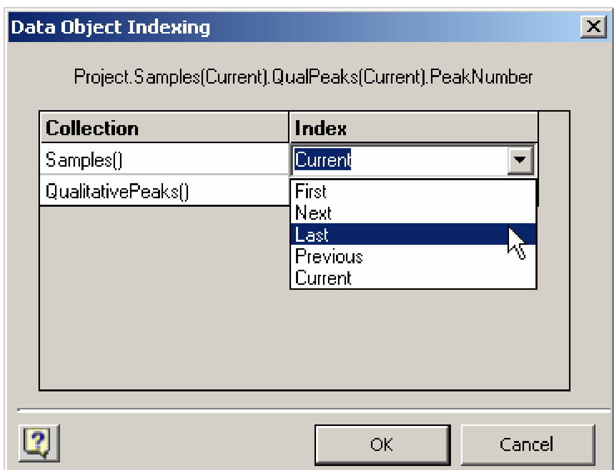
To report the most recent line in the Sample List we need to change the Indexing of the Peak Number. Right click on **Peak Number (DATA)** and select Indexing from the menu.

The *Data Object Indexing* dialog appears:



Double click on **Current** in the Samples Index cell.

The following **Index** dropdown menu appears:



Select **Last** then click **OK**.

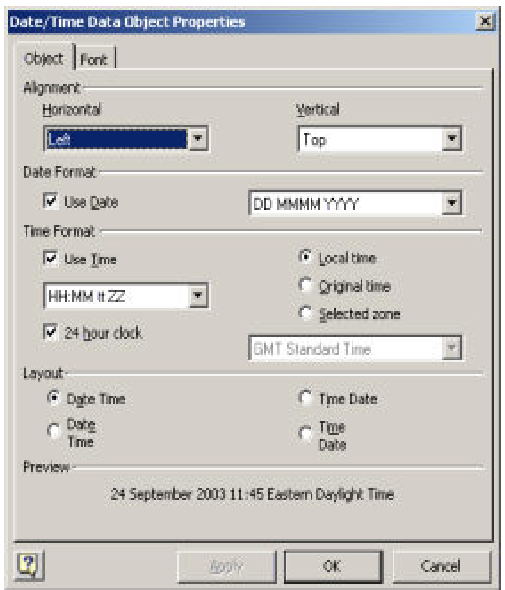
8. Under “RT” put **Retention Time**, from the Project / Samples() / Qualitative Peaks () path in the Data Objects toolbox. Set to Samples (Last).

9. Under “Name” put **Name**, from the Project / Samples() / Qualitative Peaks () path in the Data Objects toolbox. Set to Samples (Last).

10. Under “Match Factor” put **Match Factor**, from the Project / Samples() / Qualitative Peaks () / Text Hits / path in the Data Objects toolbox. Set to Samples (Last).

11. Under “Area%” put **Area%**, from the Project / Samples() / Qualitative Peaks () / path in the Data Objects toolbox. Set to Samples (Last).

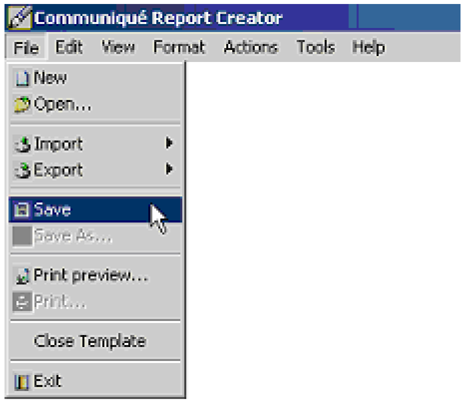
12. Check your **Date/Time Data Object Properties** for the correct **Time Format**.



The default Communiqué setting for **Date/Time Data Objects** is "**Local time**." In order to ensure that the correct time is reported on your computer, right-click the **Date/Time Object** in your template, select Object Properties from the pop-up menu and in the following dialog select "**Original time**" to set the Time Format, then click **OK**.

NOTE: *When setting the Numeric Data Object Properties in your Communique template, increase the number of significant figures from the default of 4 to 6 in order to see the reported number with no rounding applied. Otherwise Communiqué doesnot report 6 figures but instead applies rounding.*

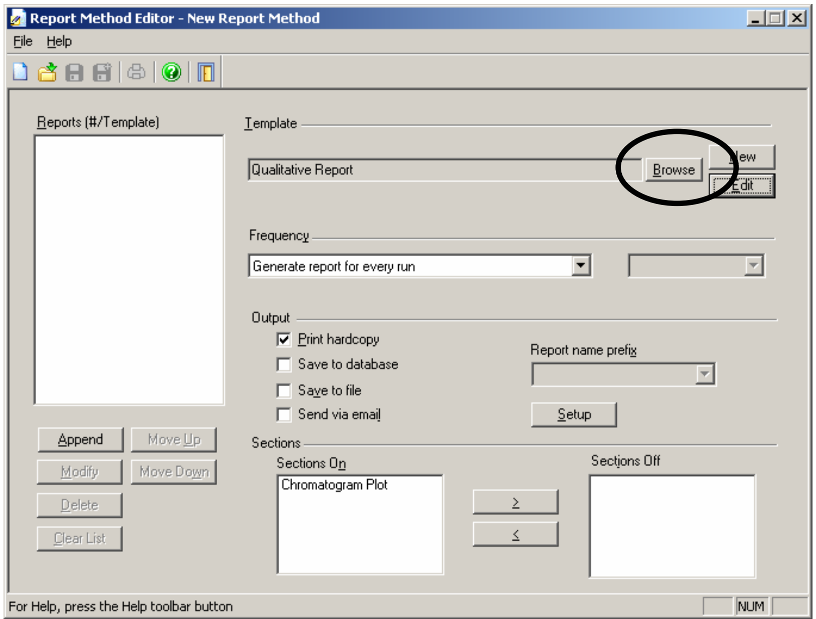
13. Select **Save** from the Communiqué Report Creator *File* menu and name the file (for example, Mod Qualitative Report).



14. Close *Communiqué Report Creator* by clicking **Exit** from the *File* menu.

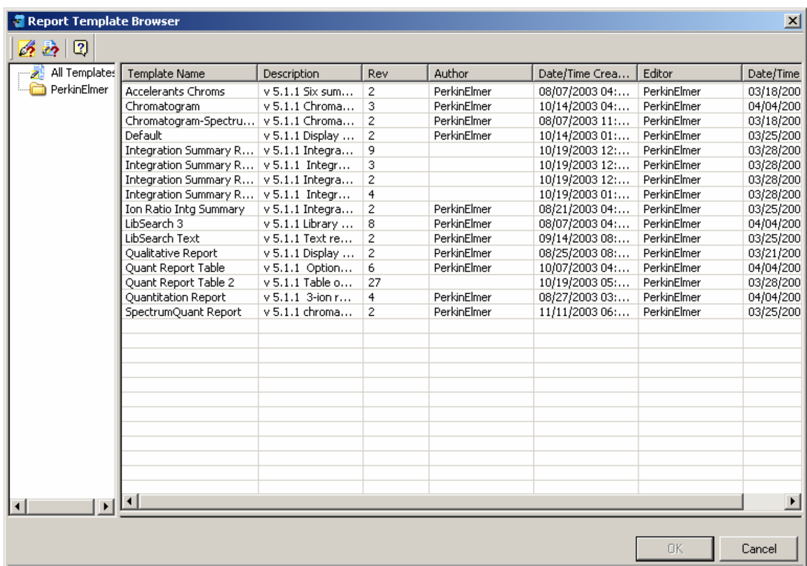
Select the Template in the Report Method Editor

After closing the *Communiqué Report Creator* the Report Method Editor appears:



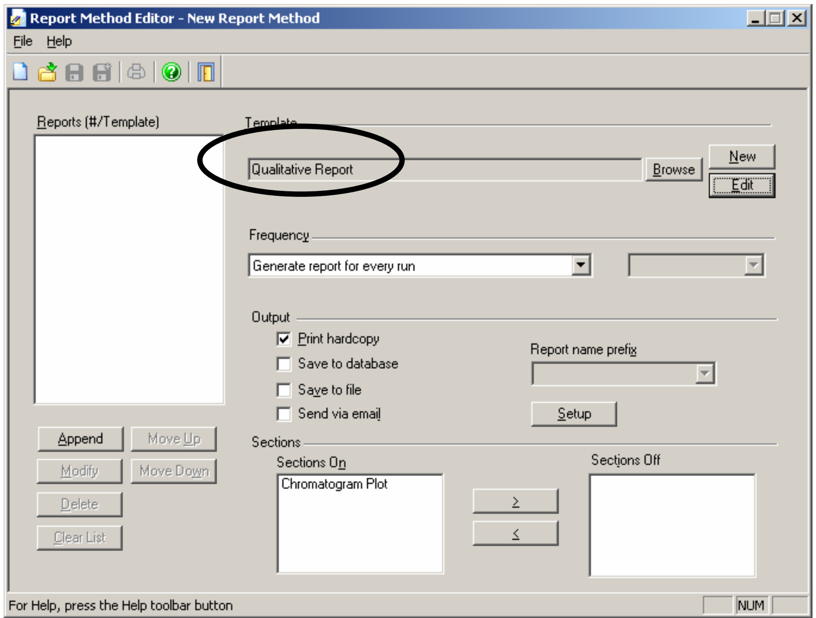
1. Click the **Browse** button.

   The following dialog appears:



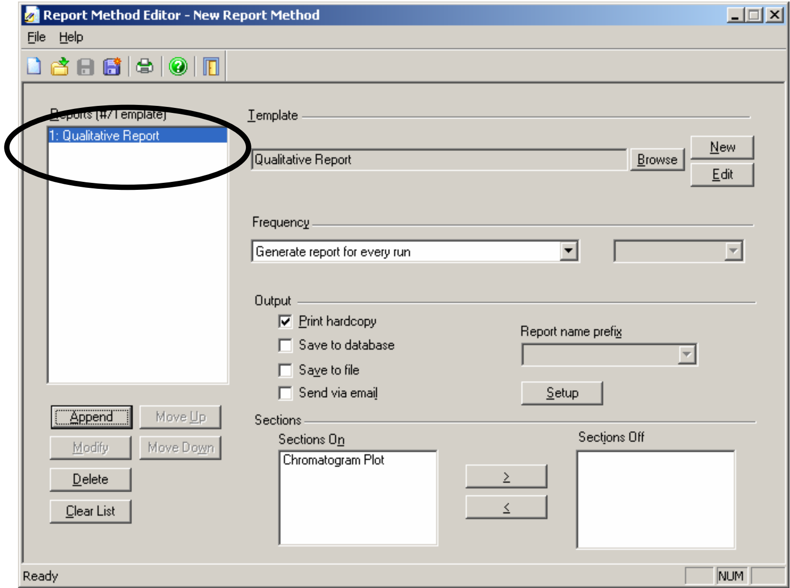
2. Select your template (for example, Qualitative Report) and click **OK**.

   Qualitative Report appears as shown below:



3. Click the **Append** button.

   This template appears in the **Report (#/Template)** field This is a display of the reports defined for the current method.



When the list is empty (New Method, after **Clear List** or after all reports have been **Deleted)** the controls on the right will be set to default values. In this way the Append button is always enabled and valid.

Using the **Move Up** and **Move Down** command buttons reorders the Reports in the list. Reports will be processed by report number (i.e. in the order in the list).

4. Set the other options on this screen. For example, set the **Frequency** to one of the following:

5. Generate report for every run.

6. Generate report for every run of specified type. (Analyte, Blank, QC, or Standard)

7. Generate report only for final row in the sample list.

8. Set the **Output** options and specify a Report name prefix if it is required by the Output type selected. (For example, if you select **Save to file**, select a Report

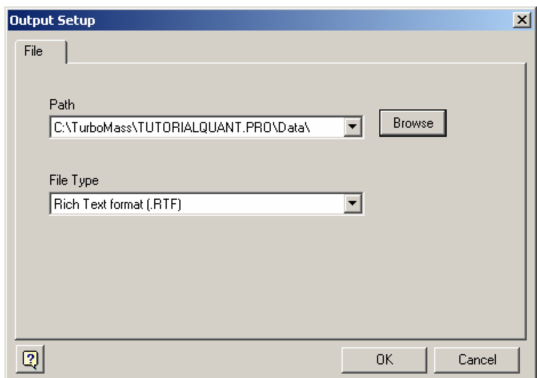
name prefix of <Sample Name>, and click the **Setup** button. This drop–down list contains the report output file types supported by Communiqué:

NOTE: *To ensure that a CSV file puts data items on the same line, enclose all items that are required to appear on one line of the CSV file in a Communiqué Section object. All items enclosed in the Section should have the 'Down from Top' property set to zero (0). Also, all items should have the same 'Height' value set as the Section itself.*

- Rich Text Format (.RTF)
- HTML (.HTM)
- ASCII Text (.TXT)
- Comma separated (.CSV)
- Portable Data Format (.PDF)
- Web Archive, Single File (.MHT)

NOTE: *The Web Archive, Single File type embeds the graphics into the same .htm as the text portion of the report resulting in a single file with both text and graphics.*

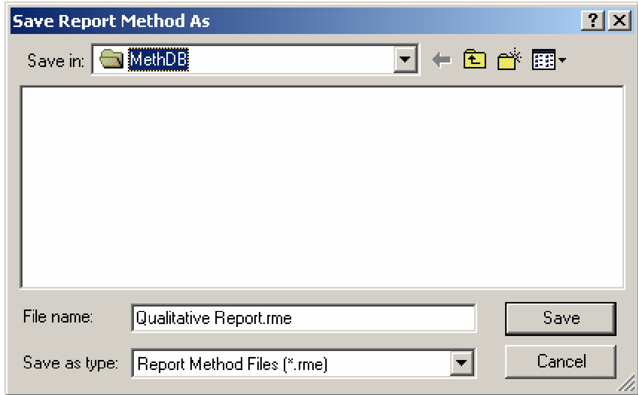
The following dialog appears:



9. Click **OK**.

10. Select **Save As** from the Report Method Editor **File** menu.

11. The **Save Report Method As** dialog appears:

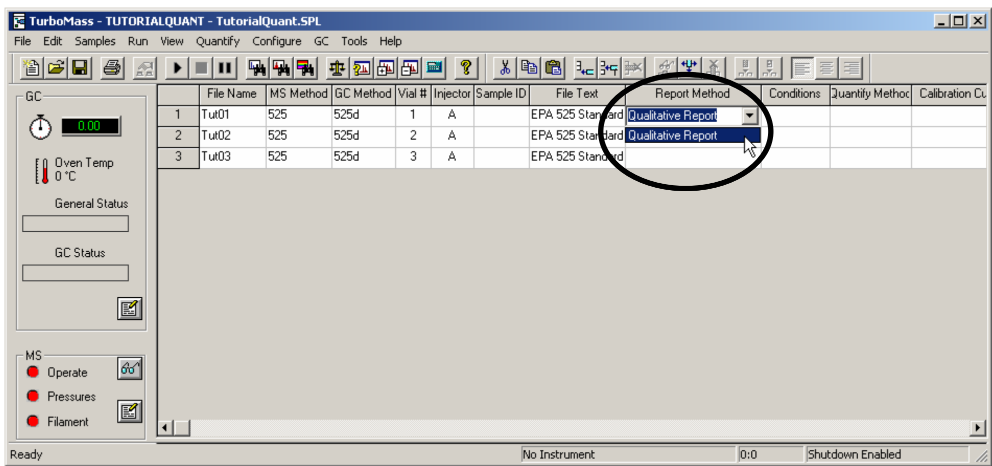


12. Type a File name for your Report Method (for example, Qualitative Report) then click **Save**.

    This Report Method is now available for the **Report Method** column of the **Sample List**.

Add the Report Method to the Sample List

1. Double-click in the **Report Method** field and select **Qualitative Method** from the drop-down list.



2. Close the Report Method Editor by clicking the Close box (in the upper-right hand corner of the screen).

Environmental Reporting 21

About Environmental Reporting

TurboMass Environmental Reporting software generates reports based on lists of PerkinElmer TurboMass and Clarus GC/MS samples (Sample List). These reports, while based on U.S. Environmental Protection Agency (US EPA) requirements, are designed to be flexible and customizable to support worldwide environmental and QA/QC reporting requirements governed by NELAC and ISO 17025.

You can add samples to the list or create new lists using either the Sample List or Sample List Wizard. While the Sample List is typically created prior to data acquisition, it can be created and edited any time prior to environmental report generation.

In the Report Generation window you can select the Forms you want printed and the data set to be used as input. Also, the selection of Tentatively Identified Compounds (TIC) from the initial library search qualitative processing is made within this environment.

IMPORTANT: *If you change the quantitative results at the report generation time (for example, you select a different method) you must reprocess, otherwise the qualifier flag assignments may be invalid.*

Report generation is a daily operation within the environmental laboratory and TurboMass Environmental Reporting is designed to streamline the process.

TurboMass Environmental Reporting supports:

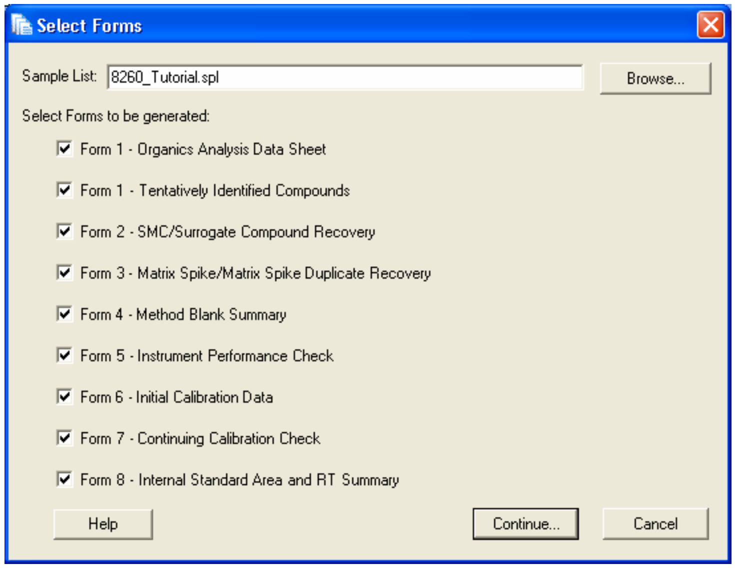
- Efficient environmental report generation based upon environmental QA/QC sample batches
- A powerful interactive data review environment
- Custom per-client and per-project compound lists
    - Automatically report only client-requested compounds
    - Does not need a new Quantify method and Calibration curve

  - Do not need to manually delete target compounds for TIC searching and reporting

- Intelligent errors and warnings report of missing information during file selection
- Intelligent default selection of files for QA/QC reports
- Optional reporting of "J" flagged-compounds
- Easy review and selection of TIC compound name results
- Easy to customize reports without programming

Select Forms Dialog

The Select Forms dialog provides you with the interface to select reports to be printed. These reports are based upon templates, or "Forms" defined by the US EPA.



The exact format of the report you generate depends upon several selections you make within the Sample List or Sample List Wizard environments. These include the following:

Sample Type

Volatiles (VOA), Semivolatiles (SV), or QA/QC

Matrix

Water or Soil

Concentration (SV only)

PerkinElmer provides two sets of reports, one based on the US EPA OLM04.2 specification ("CLP-Like), and the other (the default) a format enhanced with

additional laboratory information and with a more attractive and convenient format (PKI format).

The reports may optionally be defined by a configuration table set up by the TurboMass administrator. This table maps the specified report to a Communiqué reporting template. The table applies to the current TurboMass Project and the configuration file is copied to a new Project as part of the New Project Wizard functionality.

In TurboMass terms, the Forms are a combination of single run reports and summary reports. The Environmental Reporting environment automatically generates one or more temporary Sample Lists based upon the needs of each report, and adds them to the Communiqué report generation queue.

The normal Communiqué report generation procedures can be used to produce most of the non-summary Forms automatically after data acquisition. Non-environmental Communiqué reports (e.g. chromatogram plots, library search results, quantitation plots) can also be produced in the same manner.

The selections in the Select Forms dialog are described below:

Parameter	Description
Sample list	The name of the sample list to be processed. You type it in or select it from the current project (only) using the Browse button.
Browse...	A button, when clicked, displays a standard File Open dialog (with the Title 'Select Sample List'), allowing you to select a stored sample list (*.SPL file).
Form 1 - Organics Analysis Data Sheet	Selecting this check box indicates that Form 1 report is to be generated for each applicable sample in the sample list. Form 1 reports the concentrations of target compounds in the sample.

Form 1 - Tentatively Identified Compounds	Selecting this check box indicates that Form 1 Tentatively Identified Compound (TIC) report is to be generated for each applicable sample in the sample list. Form 1 TIC shows library search results for the largest (typically 10 to 30) non-target peaks in the. Each is assigned an estimated concentration based upon its response compared to the Total Ion Current of the nearest internal standard compound. TurboMass qualitative processing prior to entering the Select Reports window will initially generate a list of several potential hits from the NIST library search. You must choose one of these hits for each unidentified peak, enter an alternative text (e.g., long-chain hydrocarbon), or delete the TIC peak from the report. Until you have performed this task the qualitative results will be marked (in the qualitative data file) as Pending. The data file be marked Complete only after you have reviewed the data for each peak and accepted the default compound identification, or selected a different one.
Form 2 - SMC/Surrogate Compound Recovery	Form 2 reports the recoveries of the specific analytes defined as System Monitoring Compounds (SMC, also called "surrogates".) It flags any compound whose recovery is outside of Quantify Method specified limits. The sample to be used as the source of the header information for the report is indicated by the data source item 'Header Sample Index'. This defaults to the first checked (i.e., selected for processing) Analyte or Analyte Dup row in the sample list but you may reassigned this.
Form 3 - Matrix Spike/Matrix Spike Duplicate Recovery	Form 3 reports the recoveries of specific analytes defined as spike compounds in the sample; the matrix spike (MS), and the matrix spike duplicate (MSD). It flags any compound whose recovery or relative percent deviation (RSD %) is outside of the Quantify Method defined limits.

Form 4 - Method Blank Summary	Form 4 designates which samples were acquired reporting to a particular method blank.
Form 5 - Instrument Performance Check	Form 5 reports the compliance of the BFB or DFTPP tune evaluation sample (instrument performance check), and lists all data files acquired while this tune file was valid.
Form 6 - Initial Calibration Data	Form 6 reports the initial calibration of the instrument based on a multi-level calibration. The average relative response factor (RRF) and its relative standard deviation (RSD) are reported for all RRF-calibrated target compounds. It flags any compound whose response factors or relative standard deviations are outside of the Quantify Method defined limits. The r-squared correlation coefficient is calculated for linearly calibrated compounds, and the Form flags values outside of Quantify Method defined limits. You will identify a specific row in the sample list to be used as the source of the Form 6 header data. This will default to the first checked (i.e., selected for processing) Analyte or Analyte Dup row identified as referencing the calibration file to be used as the source of the Form 6 data.
Form 7 - Continuing Calibration Check	Form 7 compares the daily calibration check (continuing calibration) data against the initial calibration data of the instrument. Compounds whose relative response factors or % differences exceed Quantify Method defined limits are flagged. Linearly or quadratically calibrated compounds are flagged if their % drifts exceed Method limits.
Form 8 - Internal Standard Area and RT Summary	Form 8 reports the retention time and area reproducibility for the internal standards for all data selected.

Continue	This button opens the main environmental reports generation window.
Cancel	This button closes the Generate Forms dialog.

NOTE: *Whenever you select a new sample list and click Continue, the main environmental reports generation window will open with the Sample List tab selected. If the sample list is the same one you had previously been working with in the current session and the Select Forms dialog was only used to change Forms selected then Continue will return to the previously selected Form tab (unless this is no longer present, in which case the Sample List tab will be selected).*

Report Generation Window

In this window you can select the Forms you want printed and the Sample List(s) to be used as input. The selection of Tentatively Identified Compounds from the initial qualitative processing will also be made within this window. This window displays a comprehensive view for generating reports using the EPA Forms 1 through 8 that apply to GC/MS analyses.

The process of generating the Forms will involve the reprocessing a Sample List by the TurboMass software (as with other Communiqué reports) but there are several unique aspects in this case:

1. The Sample List is queued for reprocessing from this window rather than from the Sample List window.

2. The Start Sample List Run dialog does not appear. The reprocessing always uses the following options:

    - Auto Quantify Samples = On (Quantify Samples only)

    - Generate Communiqué Reports = On

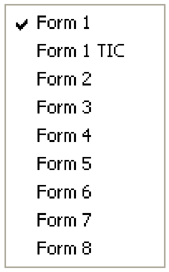
    - Quantify, Qualify, and Generate Reports = After Each Run (or summary reports at the end of the sample list)

3. Which sample rows are processed will be indicated by the user on the Sample List tab. Individual rows can be turned on or off for processing.

4. The Report Method supplied to the Report Manager (and hence the template(s) provided to Communiqué will not be that in the Report Method column of the Sample List but will instead depend on the Forms selected by the user and the Submitter and Task associated with the sample. The Report Method in the Sample List can be execute in the usual manner (Run/Start from the Sample List).

NOTE: *During the sample list processing associated with report generation, processing from within the Quantify window (View Results) will be inaccessible to a user. This is to prevent possible data file conflicts.*

Context Menu (Sample List Tab) - The following pop-up menu appears when you right–click on the Sample List tab (i.e., the label area you click on to select the tab). It allows you to quickly select and deselect Forms for printing.



Form tab - Remove This Form - Removes the tab associated with the clicked–on label from the Report Generation Window. The associated Form will not be printed.

Report Generation Window Menu

The following reporting controls are available from the Report Generation Window.

Menu Item	Command	Description
Sample List	Append Sample List…	Opens a data browser, allowing the selection of a sample list file from the current Project only. The selected sample list will be appended to the list already displayed in the window. This command is only enabled when the Sample List tab is selected.
	Save As…	Opens a Save As dialog, allowing you to enter a file name within the current Project.
	Exit	Exits the Report Generation window.

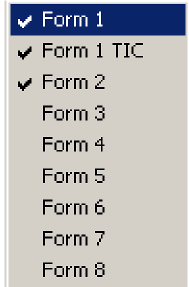
Menu Item	Command	Description
Forms	Print	Queues the selected sample list rows for reprocessing.
	Assign Tentatively Identified Compounds...	Opens the Tentatively Identified Compounds dialog. Enabled when the Form 1 TIC tab is selected and no Form 1 TIC errors exist.
	Assign Header Sample	Assigns the selected row as the source of report header information for Form 2. Displays Header in the Status column for that row.
	Assign Analyte	Assigns the selected row as the Analyte to be treated as the sample which gets spiked to produce the MS and MSD samples for Form 3. Displays **Analyte** in the Status column for that row and displays the row in the Analyte color. Enabled when the Form 3 tab is selected.
	Assign Matrix Spike Sample	Assigns the selected row as the Matrix Spike sample for Form 3. Displays **Spike** in the Status column for that row and displays the row in the Spike color. Enabled when the Form 3 tab is selected.
	Assign Matrix Spike Duplicate	Assigns the selected row as the Matrix Spike Duplicate sample for Form 3. Displays **Spike Dup** in the Status column for that row and displays the row in the Spike Dup color. Enabled when the Form 3 tab is selected.

Menu Item	Command	Description
	Assign Method Blank	Assigns the selected row as the Method Blank sample for Form 4. Displays **Meth Blank** in the Status column for that row and displays the row in the primary data color. Enabled when the Form 4 tab is selected.
	Assign Tune Evaluation Sample	Assigns the selected row as the Tune Evaluation sample for Form 5. Displays **Tune Eval** in the Status column for that row and displays the row in the primary data color. Enabled when the Form 5 tab is selected. **NOTE:** It is valid for the same row to be identified as a Tune Eval for Form 5 and a Cont Calib for Form 7.
	Assign Continuing Calibration	Assigns the selected row as the Continuing Calibration sample for Form 7. Displays **Cont Calib** in the Status column for that row and displays the row in the primary data color. Enabled when the Form 7 tab is selected. **NOTE:** It is valid for the same row to be identified as a Tune Eval for Form 5 and a Cont Calib for Form 7 [and Form 8].

Menu Item	Command	Description
	Assign Mid-Level Standard	Assigns the selected row as the Continuing Calibration (Mid–Level Calibration) sample for Form 8. Displays **Cont Calib** in the Status column for that row and displays the row in the primary data color. Enabled when the Form 8 tab is selected. **NOTE:** It is valid for the same row to be identified as a Tune Eval for Form 5 and a Cont Calib for Form 8 [and Form 7].
	Select Forms…	Displays the Select Forms dialog. If you select a new sample list within the Select Forms dialog the existing sample list will be replaced and any reassignments will be lost.
Options	Customize Display...	Opens the Customize Field Display dialog to enable you to select the columns to appear in the sample list view (Both on Sample List tab and Form–specific tabs). When the dialog is closed the display is updated. It is disabled when the Form 6 tab is displayed (since there are no selectable columns on the tab).
Help	Help Topics	Opens this TurboMass Report Generation Help window.

Sample List Context Menu

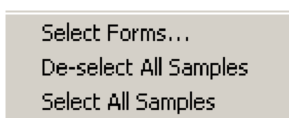
The following pop-up menu appears when you right–click on the Sample List tab itself (i.e., the area you click on to select the tab).



NOTE: *The symbol ✓ in front of an item indicates that this is an on/off toggle command. The check mark appears in front of the Form when the function is active or selected. This applies to all menus described in this document.*

Menu Item	**Description**
✓ Form X Where X is a Form number 1 through 8	Toggles display of the Form X tab. If the change is from Off to On, the error/warning checks for Form X will be performed. If the change is from On to Off any errors/warnings for Form X will be eliminated.

The following pop-up menu appears when you right–click on the Sample List view pane.



Menu Item	Description
Select Forms…	Displays the Select Forms dialog, enabling you to change the set of Forms to be generated.
De-select All Samples	Removes the checks from all boxes leaving no samples selected.
Select All Samples	Add check marks to all boxes thereby selecting all samples.

How to Generate a Report

To generate a set of environmental reports, follow this procedure:

IMPORTANT: *If you change the quantitative results at the report generation time (for example, you select a different method) you must reprocess, otherwise the qualifier flag assignments may be invalid.*

1. Choose the Environmental Reports… command from the Tools menu of the Sample List window or press the icon on the Sample List icon bar.

2. Use the default sample list (the one displayed in the **Sample List** window) or select a different one.

3. Select the set of **Forms** to be generated.

4. Review the displayed sample list and any global errors or form–specific errors identified by the TurboMass software.
   - Correct any global errors (if possible) by changing the rows selected for processing in the sample list.
   - Correct any form–specific errors (if possible) by adjusting sample assignments associated with Form.

5. Open the **Tentatively Identified Compounds** dialog (if a Form 1 TIC has been selected – or else skip to step 8) and review the default compound assignments for each reported peak.

6. As appropriate, compare the spectra of the alternate search hits with the peak spectrum and change the TIC assignment if necessary.

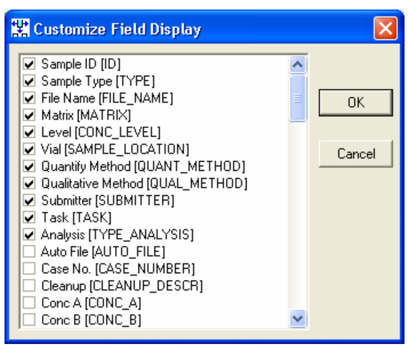
7. Close the **Tentatively Identified Compounds** dialog when all peaks have been reviewed.

8. Choose the **Print** command from the **Report** menu. The TurboMass software then queues the selected rows of the sample list for processing for all selected reports.

Customized Field Display

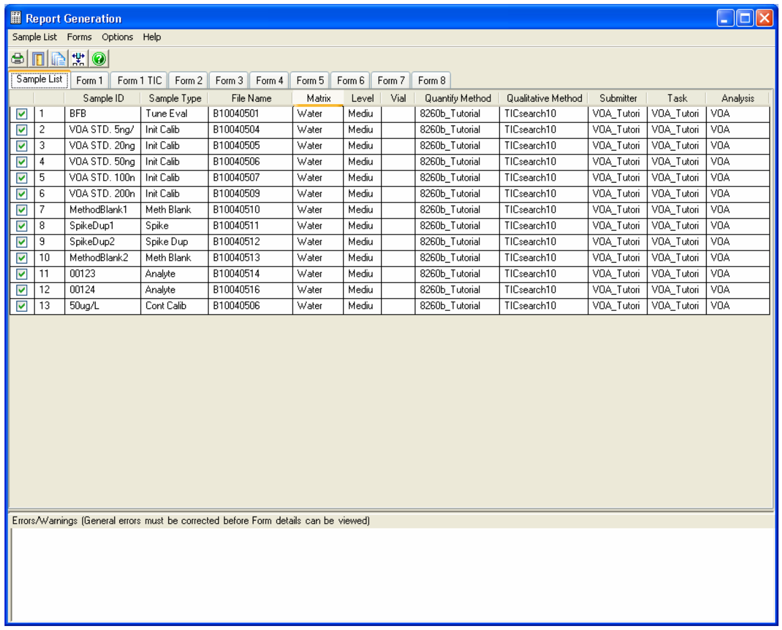
You are able to define which data columns are displayed using the Options menu item Customize Field Display dialog to appear in the sample list view (both on Sample List tab and Form–specific tabs, where applicable). The display is updated when the dialog is closed.

This dialog is disabled when the Form 6 tab is displayed (since there are no selectable columns on this tab) but enabled at all other times.



Sample List Tab

The Report Generation window is displayed when the **Continue** button is clicked in the **Select Forms** dialog. The Sample List tab is selected initially. An additional tab will display for each of the Forms selected in the **Select Forms** dialog. The following screen shows all forms selected.



Row Colors

The color in which rows are displayed indicates how they will be used in the generation of the current form.

Disregard – Gray: *Gray indicates that the row is not involved in the generation of the Form.*

Primary – Blue: *Blue indicates that the row is the primary data set for a Form. For example, multiple blue rows in the Form 1 tab indicate that a separate Form 1 will*

be generated for each row. Most other Forms have just one blue row indicating that just one Form of that type will be generated for the sample list.

Summary – Black: *Black indicates that the row will form part of a summary table on the form. For example see Form 2 or Form 5.*

Other Colors: *Form 3 is a unique case, in that it involves three (or possibly just two) files that are interrelated. Each of these three rows uses a unique color to indicate its role.*

About this Window

1. You can size this window and the relative sizes of the sample list and message panes may be adjusted using the splitter bar.

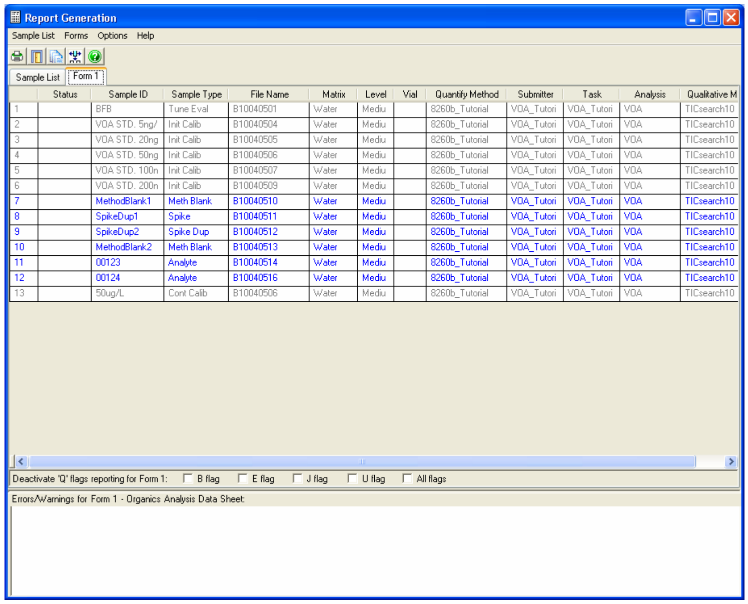
2. The first column in the list view (check box and row number) always appears but the other columns are configurable by the user in the same way as for the main TurboMass Sample List window.

3. Any rows in the sample list that do not contain a (raw data) file name will be ignored and not added to the view. (This would remove the comments added to the Tutorial Reports sample list included with the example data.)

4. The row number associated with each row in the sample list remains unchanged on all tabs. That is, if rows are unchecked on the Sample List tab then there will be gaps in the numbering on the Form tabs (which only display data files that have been selected for reporting).

Form 1 Tab – Organics Analysis Data Sheet

When you select **Form 1 - Organics Analysis Data Sheet** from the Select Forms dialog the **Report Generation Window – Form 1 Tab** appears.



Qualifiers (Q Flags)

In addition to the concentration of a compound the Form 1 also contains a column labeled "Q" for qualifier. A qualifier provides additional information about the compound.

IMPORTANT: *If you change the quantitative results at the report generation time (for example, you select a different method) you must reprocess, otherwise the qualifier flag assignments may be invalid.*

The EPA-defined qualifiers are:

U This flag indicates the compound was analyzed for but not detected or below the MDL..

NOTE: *For the purpose of environmental reports the term **MDL** is used to indicate the threshold value for the "U" qualifier flag. Values below this threshold value will flag the compound with a "U" in the Form 1 report and no concentration values will be printed.*

J This flag indicates an estimated value. This flag is used in the following circumstances:

- When estimating a concentration for Tentatively Identified Compounds where a 1:1 response to the total ion current of the nearest internal standard is assumed (Form 1 TIC)
- When the mass spectral and retention time data indicate the presence of a compound that meets the volatile and semivolatile GC/MS identification criteria, and the result is between the compound's MDL and Reporting Limit. (Form 1).

IMPORTANT: *The **Reporting Threshold** value will be used as the Reporting Limit for the purpose of Setting flags on Form 1 and determining what Compounds to show on the general environmental Quantitative Report (PKIEnvQuant template) if no Custom Compound List (which includes Reporting Limits) is defined.*

N This flag indicates presumptive evidence of a compound. This flag is only used for Tentatively Identified Compounds, where the identification is based on a mass spectral library search. It is applied to all Tentatively Identified Compounds results. For generic characterization of a Tentatively Identified Compound, such as "chlorinated hydrocarbon", the N flag is not used.

B This flag is used when the analyte is found in the associated method blank as well as in the sample. It indicates probable blank contamination and warns the data user to take appropriate action. This flag is used for a tentatively identified compound as well as for a positively identified target compound. Blank contaminants are flagged B only when they are detected in the sample.

E This flag identifies compounds whose concentrations exceed the upper level of the calibration range of the instrument for that specific analysis. If one or more compounds have a response greater than the upper level of the calibration range, the sample or extract shall be diluted and reanalyzed.

D If a sample or extract is reanalyzed at a higher dilution factor, for example when the concentration of an Analyte exceeds the upper calibration range, all reported concentrations on that Form I are flagged with the D flag. This flag alerts data users that any discrepancies between the reported concentrations may be due to dilution of the sample or extract.

A This manually-applied flag indicates that a tentatively identified compound is a suspected aldol-condensation product.

X Other specific flags may be required to properly define the results. If used, the flags should be fully described.

Section of the Window	Description
Sample List view	The spreadsheet displays selected information from the Sample List. Column widths can be changed in the standard way, by dragging the header divider. The selected columns can be changed using the Options/Customize Display.
Deactivate Q flags reporting for Form 1	This Form includes one unique feature; it contains check boxes enabling you to deactivate specific **Q flag** reporting. Any Q Flags selected will not be printed in the Q column of Form 1 for any compound. The All flags selection will prevent any Q flags from being reported.
Message pane	Shows general warnings and all form–specific errors/warnings.

NOTE: *The row numbers appearing for each sample on this tab (and all Form tabs) will be the same as those from the Sample List tab.*

Form 1 TIC Tab – Tentatively Identified Compounds

The Status column of the **Form 1 TIC** (Tentatively Identified Compounds) indicates whether or not the qualitative results have been reviewed and a Tentatively Identified Compound selected for each peak (even if this was just an implicit acceptance of the default top hit). **Pending** indicates that the file has not yet been fully reviewed, **Complete** indicates that TIC selection has been completed for the file.

NOTE: *When using TurboMass to run Environmental Reports, in the Qualitative Method Editor, 'Exclude target compounds' must be checked so that Form 1 TIC reports the proper results.*

Section of the Window	Description
Sample List view	The spreadsheet displays selected information from the Sample List. Column widths can be changed in the standard way, by dragging the header divider. The selected columns can be changed using the Options/Customize Display.
Message pane	This is a read–only display window displaying messages. Shows general warnings and all form–specific errors/warnings.

As for Form 1, the Form 1 TIC display shows all rows other than **Tune Eval** and calibration rows in the primary data color (see Row Colors), which indicates that a separate report will be generated for each row.

Context Menu

A pop-up menu appears when you right–click on the Form 1 TIC row with the following item:

Assign Tentatively Identified Compounds... - This opens the Tentatively Identified Compounds dialog which allows you to match peaks with compound names.

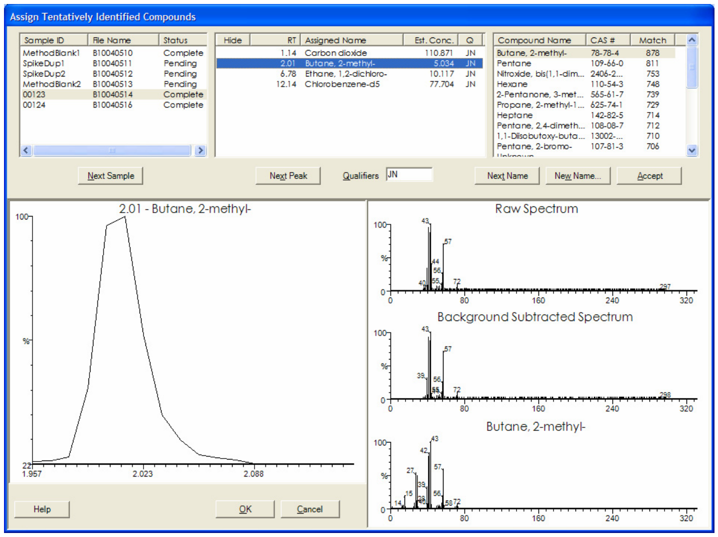
About Tentatively Identified Compounds

This dialog displays when you choose the **Assign Tentatively Identified Compounds...** command from the **Forms** menu (or the context menu on the Form 1 TIC tab). In this dialog you review the hits for the set of unidentified peaks from each sample run (excluding tune evaluation and calibration samples) and assign a compound name to each peak. In addition to the specific compound names supplied from the NIST library search you have access to a set of generic terms (such as *unknown alkane*, *unknown aromatic*) created previously by an administrator.

A typical session of assigning TICs might involve selecting names to be applied to each of 10 to 20 peaks from 20 or more samples. This list of TICs must be previously generated in the Sample List window using a qualitative method.

If the NIST library search has done a good job it may be possible to simply accept all the default compounds names offered (i.e., the highest rated hit). For this reason the software provides for a simultaneous display of the *current tentatively identified compound* setting for each peak in a selected sample. This display also allows reviewing the final set of selections to ensure consistency, e.g., the same compound name has not been used twice).

The following screen is a general layout of the Tentatively Identified Compounds dialog prior to your interaction (other than selecting a file).



Parameter	Description
File list	This list displays the files for which TICs must be identified. It also displays the TIC status as Pending or Complete.

Sample ID - The Sample ID field from the selected sample list row (this can be left empty)

File name - The raw file name for the selected sample row (this cannot be left empty)

Status - Indicates whether or not the TIC names have been reviewed for each sample row

When an unreviewed file is selected (directly or using the Next Sample button) the peak list associated with that file will be displayed in the center list, with the first peak selected.

A single row in the list can be selected, which causes the peaks from the associated qualitative file to be displayed in the peak list, along with the current TIC name associated with each.

Peak list

This list view displays the peaks from the selected file that require a TIC assignment.

Del - Contains an "X" if the peak will be deleted from the report

RT - The peak retention time

Assigned Name - The currently assigned TIC name for the peak (best spectral match originally)

Est. Conc. - The estimated concentration of the compound based on the ratio of its total ion current area to that of the nearest internal standard.

Qualifiers - EPA qualifier codes assigned to the peak ('J' and 'N' originally)

When a peak is selected (directly or using the 'Next Peak' button) the library search hits associated with that peak will be displayed in the right–hand list.

The Assigned Name field will display the current compound name associated with the selected peak. The first time the peak is selected that will be the top hit from the right–hand list. Subsequently the Assigned Name will be that selected by the user (which may also be the top hit).

A single row in the list can be selected, which causes the library search results from the associated qualitative file to be displayed, along with predefined 'generic' compound names list.

Compound list	This list view displays the top hits from the library search with a predefined generic compound list at the bottom. **Compound Name** - The names from the plot hits list, plus the generic names. **CAS #** - The Chemical Abstracts Service number for the compound (for NIST hits only) **Match -** The Match factor for this compound, as returned by the NIST library search A single row in the list can be selected, which causes that compound name to be assigned to the currently selected peak and displayed in the 'Assigned Name' column for that peak. If the selected item is one of the predefined 'generic' names and the current Qualifier string contains the 'N' flag, the 'N' will be eliminated from the string.
Qualifiers	A text box indicating the EPA qualifier codes applied to the selected peak. This field is enabled when a peak is selected in the peak list and you have permission to edit qualifier codes.
Next Sample (below file list)	Click this button to mark the currently selected file as Complete and select the next file in the list.
Next Peak (below peak list)	Click this button to select the next peak in the currently selected file. If the current peak is the last in the file, then current file will be marked Complete and the next file will be selected in the file list and the first peak from that file will be selected in the peak list.
Next Name	Click this button to select the next compound name from the compound list. If this is one of the NIST plot hits then its spectrum will be displayed in the bottom spectrum control.
New Name	Click this button to display the Generic TIC Names dialog.

Accept	A command button that assigns the currently selected name in the right–hand list to the selected peak. That name will then appear in the center list in the 'Assigned Name' column.
PEAK plot	A plot of the currently selected chromatographic peak. Plot properties can be changed for this and all other plots by selecting Properties from the right-click context menu. Behavior is similar to the TurboMass Chromatogram window.
SPECTRUM	The apex spectrum from the currently selected peak
(top)	Plot properties can be changed by selecting Properties from the right-click context menu. Behavior is similar to the TurboMass Chromatogram window.
SPECTRUM (middle)	The background subtracted spectrum from the currently selected peak. Background subtraction is performed automatically using the Chromatogram Combine function. The three peak apex spectra are averaged, and the spectrum of the scan just before the beginning of the peak is subtracted.
LIBRARY SPECTRUM (bottom)	The library reference spectrum for the currently selected plot hit from the compound list. This plot is empty when one of the 'generic' compound names is selected.
OK	Click this button to close the dialog and save the set of selected compound names with each file marked Complete. If the last file in the list is selected (peaks displayed in the peak list) but not yet marked 'Complete', it will be changed to 'Complete'.
Cancel	Click this button and a message box with the message "Save changes?" plus Yes/No/Cancel buttons appears. If you click the Yes button, the set of selected compound names for each peak will be saved and the dialog closed. Clicking the No button causes no data to be saved and the dialog closes. If you click the Cancel button the dialog will remain open (but no data saved)

To assign the tentatively identified compounds for the selected files:

1. Review the displayed peak plot and spectra associated with the first peak in the selected file (and the spectrum for the top hit).

2. Click **Next Name** (or click on another name in the right–hand list) to display the spectrum associated with another plot hit compound.

3. When you have decided which compound name should be assigned to the selected peak, select that name and click **Accept**.
   or
   Having decided that none of the compound names from the plot hits list can be definitely assigned to the peak, select one of the generic names supplied
   or
   Having decided that none of the generic names is applicable either, click the New Name button and enter a new generic name for selection.

   or

   Right-clink on the current peak's retention time and select Hide/Show. This will place an "X" under the Del(eted) column and the peak will not be reported.

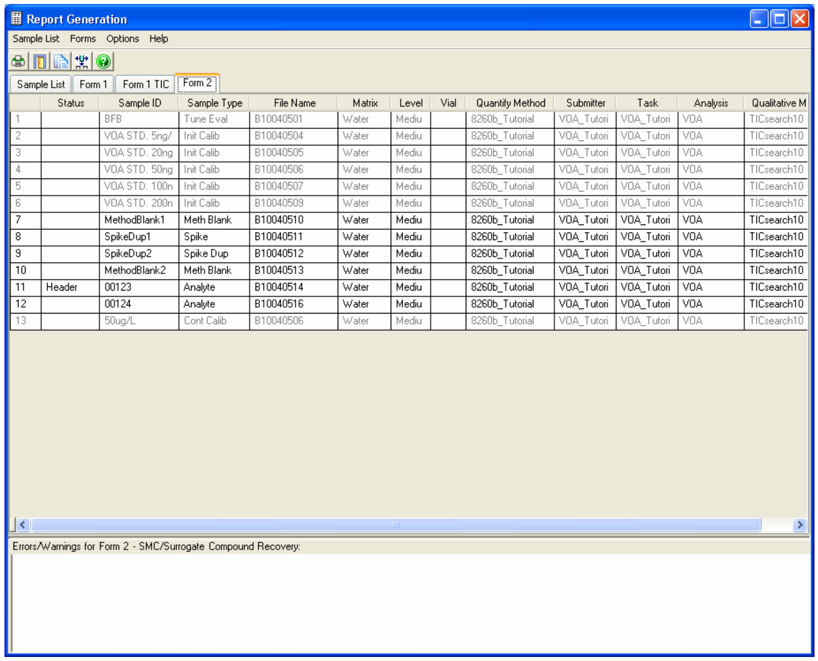
4. Edit the qualifier codes applied to the peak, if required. (The TurboMass software will automatically change the codes if a generic name is selected – see the Behavior table.)

5. Click **Next Peak**, or select another peak, or click **Next Sample** to review peaks from the next file.

6. Click **OK** after reviewing the files and changing the TIC assignments as required, to save all assignments and close the dialog. Or you can click Cancel to abandon the procedure without saving changes to the data.

Form 2 Tab - SMC/Surrogate Compound Recovery

When you select **Form 2 - SMC/Surrogate Compound Recovery** from the Select Forms dialog the **Report Generation Window – Form 2 Tab** appears with the files displayed in the summary data color.



Section of the Window	Description
Sample List view	This is a read–only display. The view cannot be sorted and no data item in any cell can be directly edited. Column widths can be changed in the standard way, by dragging the header divider. The selected columns can be changed using the Options/Customize Display.
Message pane	This is a read–only display window. Shows general warnings and all form–specific errors/warnings

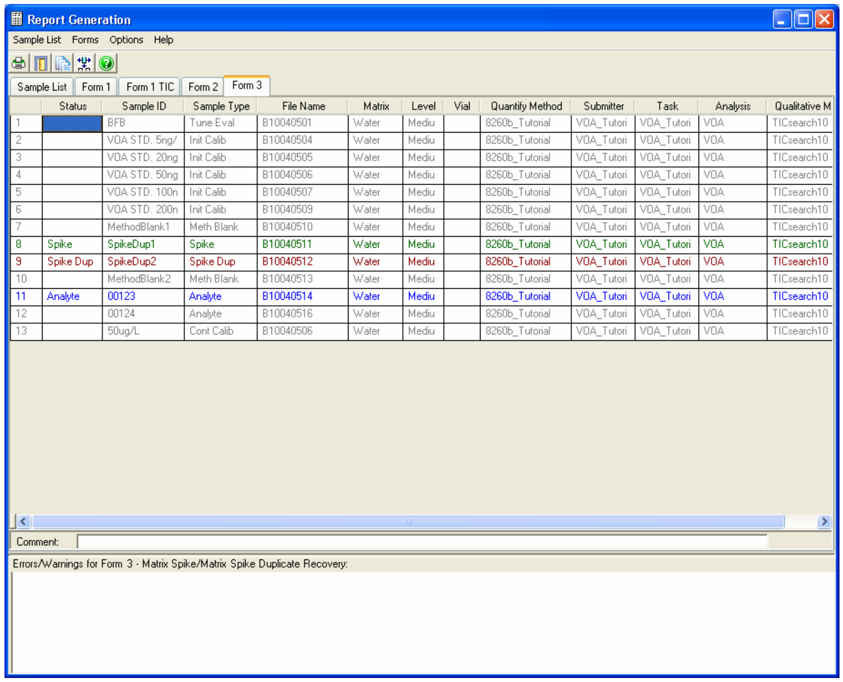
Context Menu

A pop-up menu appears when you right–click on a row (any cell) of the table containing the following item.

Assign Header Sample - If the row is an active one, it assigns the selected row as the source of report header information for Form 2. It displays Header in the Status column for that row (and eliminates Header from any other row). Inactive rows (displayed in gray) cannot be selected.

Form 3 Tab - Matrix Spike/Matrix Duplicate Recovery

When you select **Form 3 - Matrix Spike/Matrix Duplicate Recovery** from the Select Forms dialog the **Report Generation Window – Form 3 Tab** appears.



Section of the Window	**Description**
Sample List view	This is essentially a read–only display. No data item in any cell can be directly edited. Column widths can be changed in the standard way, by dragging the header divider. The view cannot be sorted.
Comment	You may enter up to 120 characters which will be printed on the report.
Message pane	This is a read–only display window. Shows general warnings and all form–specific errors/warnings

Row Colors

Form 3 shows primary data file in blue, which represents the unspiked sample analysis. It also uses two unique colors (dark green and dark red) to indicate the **Matrix Spike** sample and the **Matrix Spike Duplicate** samples. All the remaining rows are unused for the report and shown in the grey **Disregard** color.

Status Column

The Status column indicates which rows are currently flagged as the **Analyte**, **Spike** and **Spike Dup** samples to be used in generating Form 3. This apparent duplication with the Sample Type column is because it will be possible for you to over–ride the Sample List's file Type and assign a different row as one of the three key data files.

Context Menu

A pop-up menu appears when you right–click on a row in the Form 3 sample list view pane. These selections allow you to reassign the **Matrix**, **Matrix Spike**, and **Matrix Spike Duplicate** samples without returning to the Sample List. (Note that any reassignments made here are lost after the reports are printed.

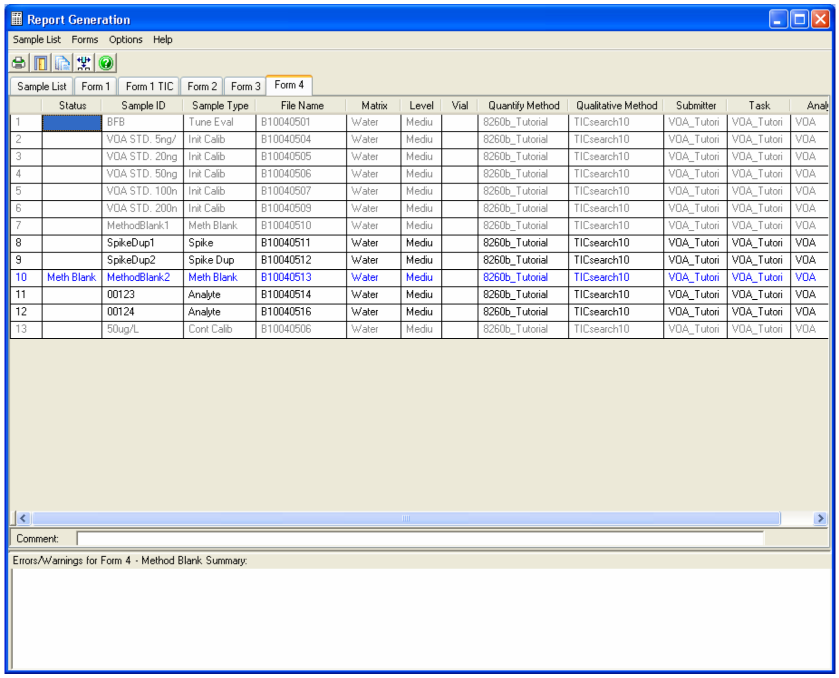
Assign Analyte - Assigns the selected row as the **Analyte** to be treated as the sample from which the MS/MSD sample are prepared for Form 3. Displays **Analyte** in the Status column for that row and displays the row in the **Analyte** color.

Assign Matrix Spike Sample - Assigns the selected row as the **Matrix Spike** sample for Form 3. Displays **Spike** in the Status column for that row and displays the row in the Spike color.

Assign Matrix Spike Duplicate - Assigns the selected row as the Matrix Spike Duplicate sample for Form 3. Displays **Spike Dup** in the Status column for that row and displays the row in the **Spike Dup** col.

Form 4 Tab - Method Blank Summary

When you select **Form 4 - Method Blank Summary** from the Select Forms dialog the Report Generation Window – Form 4 Tab appears:



Section of the Window	Description
Sample List view	This is a read–only display. The view cannot be sorted and no data item in any cell can be directly edited. Column widths can be changed in the standard way, by dragging the header divider.
Comment	You may enter up to 120 characters which will be printed on the report.
Message pane	This is a read–only display window. Shows general warnings and all form–specific errors/warnings

Row Colors

Form 4 uses the primary data file data color (see Row Colors), for the method blank (Meth Blank) sample. Any Tune Eval, Cont Calib, Init Calib or additional Meth Blank rows will be shown in the disregard color since they are not included in Form 4. All remaining rows will be shown in the summary color, indicating they will be included in the summary section of the printed report.

Status Column

The Status column indicates which row is currently flagged as the method blank. This may be used to distinguish between several Meth Blank rows in the sample list (only one can be treated as the primary data set for Form 4) or to flag a row of another Sample Type as being the method blank.

Reassign Sample Type

The software allows the Method Blank assignments to be altered without going back to the Sample List. The basic procedure is the same for all forms (where appropriate):

1. Select the tab associated with the Form for which a primary data set will be changed
2. Select the sample list row which is to become the new primary data set
3. Right-click on that row and select the required assignment

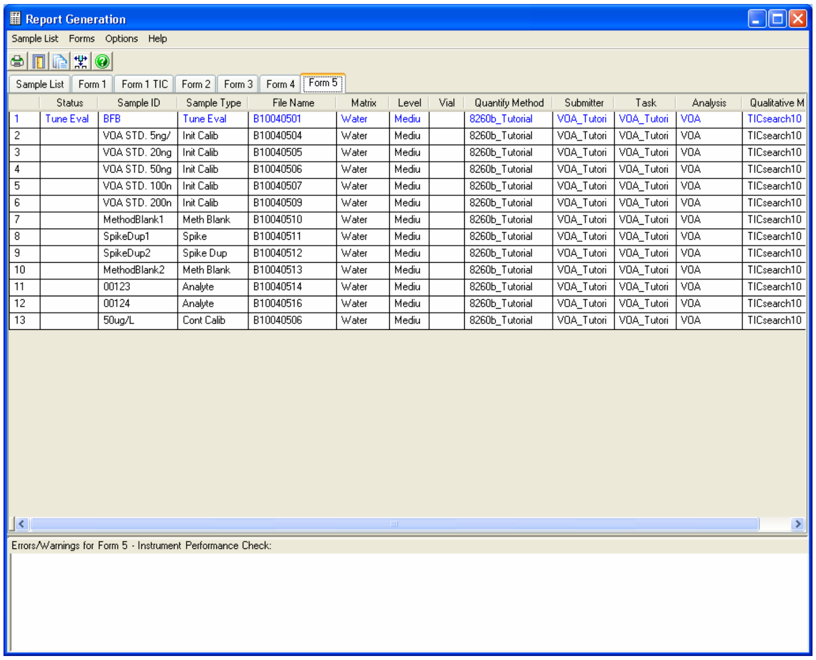
Context Menu

This pop-up menu appears when you right–click on a row in the Form 4 sample list view pane.

Assign Method Blank - Assigns the selected row as the Method Blank sample for Form 4. Displays Meth Blank in the Status column for that row and displays the row in the primary data color.

Form 5 Tab - Instrument Performance Check

When you select **Form 5 Instrument Performance Check** from the Select Forms dialog the **Report Generation Window – Form 5 Tab** appears.



Section of the Window	Description
Sample List view	This is a read–only display. The view cannot be sorted and no data item in any cell can be directly edited. Column widths can be changed in the standard way, by dragging the header divider.
Message pane	This is a read–only display window that shows general warnings and all form–specific errors/warnings.

Row Colors

Form 5 uses the primary data color (see Row Colors), represent the tune evaluation (Tune Eval) sample (BFB/DFTPP). Any additional Tune Eval rows will be shown in the disregard color. All other sample type rows will be shown in the summary color and printed on the report.

Status Column

The Status column indicates which row is currently flagged as the tune evaluation sample. This may be used to distinguish between several Tune Eval rows in the sample list (only one can be treated as the primary data set for Form 5) or to flag a row of another Sample Type (e.g. the Continuing Calibration) as being the tune evaluation sample

Reassign Sample Type

The software allows the Tune Eval assignments to be altered.

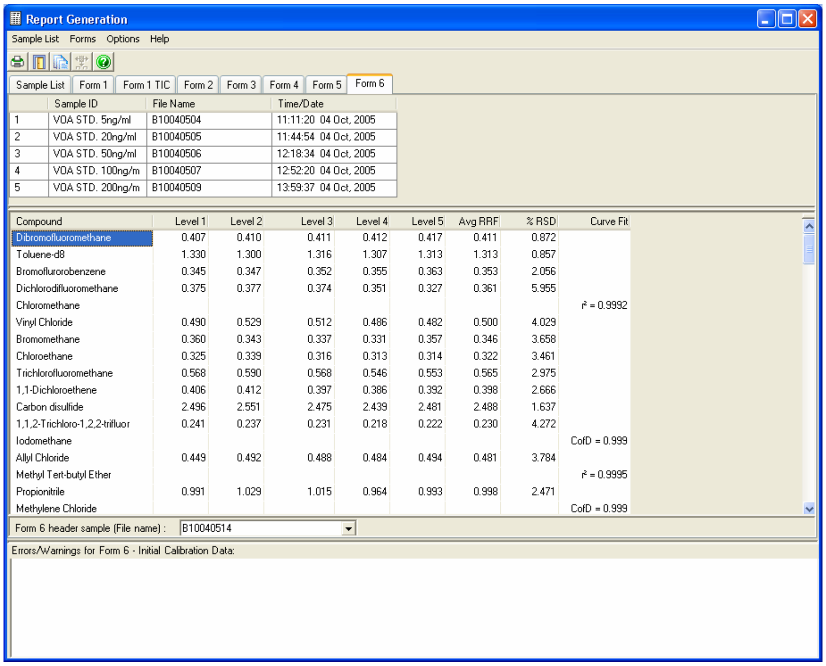
Context Menu

This pop-up menu appears when you right–click on a row in the Form 5 sample list view pane.

Assign Tune Evaluation Sample - Assigns the selected row as the Tune Evaluation sample for Form 5. Displays Tune Eval in the Status column for that row and displays the row in the primary data color.

Form 6 Tab – Initial Calibration Data

The **Form 6 tab - Initial Calibration Data** has a unique layout among the Forms. It consists of three adjustable–size panes; the calibration sample table, the compound data table and the message window.

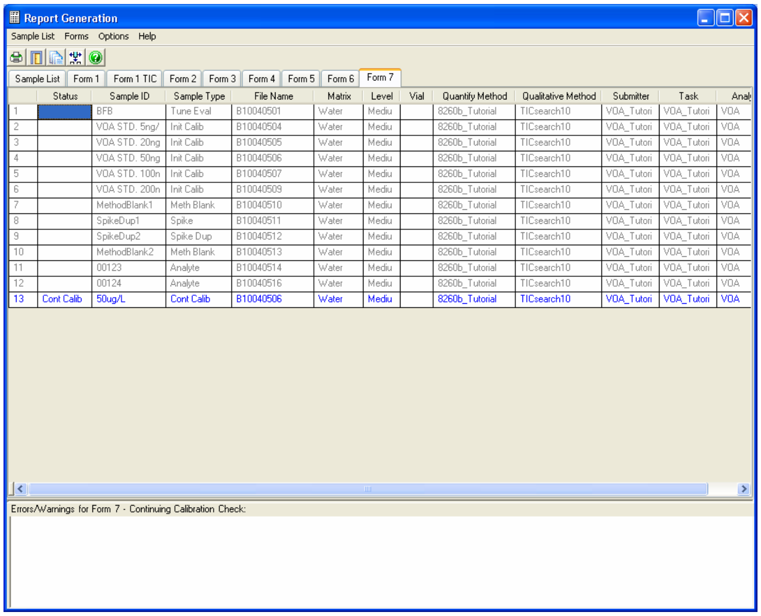


Section of the Window	Description
Calibration Sample Table	The table lists all the initial calibration data files identified in the calibration file. The table includes columns for: • Row number • Sample ID • File Name (the raw file name) • Time and date of injection of the standard sample The data for this table is taken from the first Calibration file referenced by the selected lines of the Sample List. When a row is selected the arrow keys can be used to change the selected row and cause the list to scroll. Column widths can be changed in the standard way, by dragging the header divider
Compound Data Table	The data for this table are also taken from the Calibration file. The table lists all compounds identified in the calibration file and displays the RRF value calculated for each concentration level, plus the average RRF and the percentage relative standard deviation for the RRF values. For compounds using a linear or higher-order curve fit calibration in place of Average RRF, the goodness of fit value (r^2 correlation coefficient for first order, coefficient of determination (CofD) for higher orders). RRF values flagged as below the minimum required value for that compound (as defined in the Quantify method) will be displayed in red. Similarly if the average RRF value is below the minimum required value or the %RSD value for a compound is greater than the specified maximum value for that compound, they will be displayed in red..

Section of the Window	Description
Form 6 Header sample	This drop–down list enables you to indicate the source of the information that will appear in the Form 6 header. Note that this information is not related to the calibration standard samples but rather the samples analyzed utilizing the calibration. This means that in general the source of the header information will be one of the Analyte samples from the Sample List tab. The drop–down list contains the file names of all the checked samples from the Sample List tab. The initial selection will be the first checked Analyte (or Analyte Dup) row from the Sample List tab.
Message pane	This displays errors and warnings associated with Form 6, in a similar manner to that for all other Forms.

Form 7 Tab – Continuing Calibration Check

When you select **Form 7 - Continuing Calibration Check** from the Select Forms dialog the **Report Generation Window – Form 7 Tab** appears.



Section of the Window	**Description**
Sample List view	This is a read–only display. The view cannot be sorted and no data item in any cell can be directly edited. Column widths can be changed in the standard way, by dragging the header divider.
Message pane	This is a read–only display window. Shows general warnings and all form–specific errors/warnings

NOTE: *If you change the Min RRF value in the Quantify method you must reprocess (recalibrate) the sample list for this new value to display in the report.*

Row Colors

Form 7 uses a single data file in the primary data color (see Row Colors), for the continuing calibration (Cont Calib) sample. All other rows will be shown in the disregard color and are not used for the report.

Status Column

The Status column indicates which row is currently flagged as the continuing calibration sample. This may be used to distinguish between several Cont Calib rows in the sample list (only one can be used for Form 7) or to flag a row of another Sample Type as being the continuing calibration sample.

Reassign Sample Type

The software allows the continuing calibration file assignments to be altered.

Context Menu

This pop-up menu appears when you right–click on a row in the Form 7 sample list view pane.

Assign Continuing Calibration - Assigns the selected row as the Continuing Calibration (Cont Calib) sample for Form 7. Displays Cont Calib in the Status column for that row and displays the row in the primary data color.

Form 8 Tab – Internal Standard Area and RT Summary

When you select Form 8 - Internal Standard Area and RT Summary from the Select Forms dialog the **Report Generation Window – Form 8 Tab** appears.

Section of the Window	Description
Sample List view	This is essentially a read–only display. The view cannot be sorted and no data item in any cell can be directly edited. Column widths can be changed in the standard way, by dragging the header divider.
Message pane	This is a read–only display window. Shows general warnings and all form–specific errors/warnings.

Row Colors

Form uses the primary data color (see Row Colors), for the continuing calibration (**Cont Calib**) sample. Any **Tune Eval**, **Init Calib** or additional **Cont Calib** rows will be shown in the disregard color since they are not included in Form 8.

Status Column

The Status column indicates which row is currently flagged as the continuing calibration sample. This may be used to distinguish between several **Cont Calib** rows in the sample list (only one can be treated as the primary data set for Form 8) or to flag a row of another Sample Type as being the continuing calibration sample.

Reassign Sample Type

The software allows the Method Blank assignments to be altered without going back to the Sample List.

Context Menu

A pop-up menu appears when you right–click on a row in the Form 8 sample list view pane.

Assign Mid–Level Standard - Assigns the selected row as the Mid–Level Standard (labeled as type **Cont Calib**) sample for Form 8. Displays **Cont Calib** in the Status column for that row and displays the row in the primary data color.

Error Messages and Warnings

The list of samples in Environmental Reports is checked when it is opened and whenever the rows are added or the state of any row is changed. All selected rows of the sample list are examined to identify errors or warnings. If any errors are identified then the Sample List title of the tab is displayed in red and all Form tabs are disabled. General errors and warnings are displayed in the message pane located on the bottom of the window.

Error Messages

An error is defined as a condition that will prevent the generation of a coherent data set for reporting. The Print command remains disabled while such errors exist. The following checks are made:

1. All sample rows must reference the same Analysis type (VOA, SV or QA/QC). If more than one Analysis type is present (empty Analysis fields will be ignored for this test) an error message will be displayed:
   General Error Sample list contains mixed Analysis types Rows, a, b, x-z

2. All sample list rows selected for processing, other than Tune Eval types, must reference the same Calibration file. If more than one Calibration file is referenced an error message will be displayed:
   General Error Sample list contains more than one Calibration file Rows a, b, xz

3. If no Calibration file is included in the sample list rows selected for processing, then an error message will be displayed:
   General Error No Calibration file is defined Rows az

4. All sample list rows selected for processing, other than Tune Eval types, must reference the same Quantify Method. If more than one Quantify Method is referenced an error message will be displayed:
   General Error Sample list contains more than one Quantify Method file Rows a, b, xz

5. If no selected rows reference environmental sample types (e.g. all set to Standard) an error message will be displayed:
   General Error Sample list contains no environmental sample types

6. All sample list rows selected for processing that specify a matrix type must specify the same type, or an error message will be displayed:
   General Error Sample list contains mixed matrix types Rows a, b, xz

7. All sample list rows selected for processing that specify a concentration level (low/med) must specify the same level, or an error message will be displayed:
   General Error Sample list contains mixed matrix concentration levels Rows a, b, xz

8. A sample list row selected for processing cannot be reassigned as different sample types on different Form tabs, with the exception of Tune Eval (Form 5) and Cont Calib (Form 7) [or Form 8], which is valid. For example assigning the same row as Meth Blank for Form 4 and as Tune Eval for Form 5 would cause an error message to be displayed:
   General Error Sample list contains invalid multiple sample type assignments Rows a, b, xz

9. If the calibration file identified in the sample list does not exist in the Project CurveDB directory then an error message will be displayed:
   General Error Calibration file cannot be found Rows az

10. Selected rows, other than Tune Eval or Calib types, must contain values for Analysis and Matrix.
    General Error Sample list contains sample rows with blank Analysis or Matrix column Rows az

11. If Matrix is Soil,then the Conc Level column cannot be blank.
    General Error Sample list contains Soil sample with blank Conc Level column Rows az

NOTE: *For items 1 to 5, the display of row numbers exhibiting the error is determined in one of the two following ways:*

1. The first Calibration file, Quantify Method, etc located (ignoring any referenced by the Tune Eval sample) will be taken as the correct one and any row that references a different one will be flagged as in error.

2. The Calibration file, Quantify Method, etc that is referenced most frequently in the selected rows will be taken as the correct one and any row that references a different one will be flagged as in error.

Contiguous groups of rows will be displayed in the form xz, while isolated rows will displayed separated by commas.

General errors must be cleared before the report generation process can proceed. Although general errors can be cleared by unchecking rows this may leave a sample list that cannot be used to generate the required forms (i.e., Form specific errors may be generated in the process). In this event you may have to leave this environment and edit the sample list or create a new one before generating reports.

Warnings

A warning is defined as a condition that <u>does not</u> meet the strict rules of CLP reporting but may be valid in the context of "CLP–like" reporting. Warnings do not prevent access to the Form tabs nor do they prevent reports being generated, although there is no guarantee the results will be complete or entirely valid. The following checks are made:

1. If sample list rows selected for processing specify a sample type other than one of those <u>listed</u> (plus Analyte), a warning message will be displayed: **General Warning Sample list contains nonenvironmental sample types Rows a, b, xz**

NOTE: *The display of row numbers exhibiting the warning should be determined as described in the previous section.*

2. A sample list row selected for processing should not be reassigned as different sample types on different Form tabs, with the exception of Tune Eval (Form 5) and Cont Calib (Form 7) [or Form 8], which is valid. For example assigning the same row as Meth Blank for Form 4 and as Tune Eval for Form 5 would cause a warning message to be displayed: **General Warning Sample list contains invalid multiple sample type assignments Rows a, b, xz**

3. If the injection time of any rows selected for processing is more than 12 hours after the injection time of the tune evaluation sample.

Form Specific Checks

The sample list is checked when it is opened and whenever the state of any row is changed. All selected rows of the sample list will be examined to identify errors or warnings. If any errors related to a specific Form are identified then the title of that Form tab will be displayed in red. The error will be displayed in the message pane on the Form tab as well as on the Sample List tab. Form-specific warnings will also be displayed in both places.

Form–specific errors/warnings follow General errors/warning in the message pane on the Sample List. A Form–specific error is defined as a condition that will prevent the generation of that Form. The Print command will remain disabled while such errors exist.

A Form–specific warning is defined as a condition that does not meet the strict rules of CLP reporting but may be valid in the context of "CLP–like" reporting. Warnings do not prevent reports being generated, although there is no guarantee the results will be complete or entirely valid.

Form 1

The sample list is checked for the existence of sample types reported on Form 1.
Errors: If no rows selected for processing are of sample type other than Tune Eval, Init Calib or Cont Calib then an error message will be displayed:
Form 1 Error Sample list contains no sample types reported on Form 1

Form 1 TIC

The sample list is checked for the existence of sample types reported on Form 1 TIC.
Errors:
If any rows selected for processing (of sample type other than Tune Eval, Init Calib or Cont Calib) have no associated qualitative results saved, then an error message will be displayed: **Form 1 TIC Error No qualitative data found for some selected samples Rows a, b, x–z**

If no rows selected for processing are of sample type other than Tune Eval, Init Calib or Cont Calib then an error message will be displayed: **Form 1 TIC Error Sample list contains no sample types reported on Form 1 TIC**
Either of these errors will prevent the TIC assignment process being performed.

> **Warnings: If any rows selected for processing (other than Tune Eval, Init Calib or Cont Calib rows) still have the Pending status then an error message will be displayed:** Form 1 TIC Warning Samples with incomplete TIC selection will not be reported Rows a, b, x–z

Form 2

The sample list is checked for the existence of sample types reported on Form. The first Analyte (or Analyte Dup) row found in the selected rows will be marked as the source of the header information for Form 2. You can change this assignment if necessary.
Errors: If no rows selected for processing are of sample type other than Tune Eval, Initi Calib or Cont Calib then an error message will be displayed: **Form 2 Error Sample list contains no sample types reported on Form 2**
Warnings: No warnings specific to Form 2 have been identified.

Form 3

Generation of Form 3 requires three (and only three) files: An Analyte sample, a Matrix Spike sample (prepared by spiking the analyte) and a Matrix Spike (a second spiked sample). The default rows are identified as follows:

Matrix Spike Duplicate:

- Look for the last Spike Dup sample in the list. If no Spike Dup can be located a warning condition exists (see below).

Matrix Spike:

- If a Spike Dup was located and its Sample ID ends with MSD, look for the Spike sample with the same root Sample ID but ending with MS. If this is not located, look for the first Spike sample preceding the Spike Dup. If one is not found look for the first Spike sample

following the Spike Dup. If no Spike can be located an error condition exists (see below).

- If a Spike Dup was located and its Sample ID did not end with MSD look for the first Spike sample preceding the Spike Dup. If one is not found look for the first Spike sample following the Spike Dup. If no Spike can be located an error condition exists (see below).
- If no Spike Dup was located, look for the last Spike sample in the sample list. If no Spike can be located an error condition exists (see below).

Analyte:

- If a Spike Dup was located and its Sample ID ends with MSD, look for the Analyte sample with the Sample ID formed by removing the MSD (i.e. same root, no suffix). If this is not located, look for the first Analyte (or Analyte Dup) sample preceding the Spike Dup. If one is not found look for the first Analyte (or Analyte Dup)sample following the Spike Dup. If no Analyte (or Analyte Dup) can be located an error condition exists (see below).
- If a Spike Dup was located and its Sample ID did not end with MSD look for the first Analyte (or Analyte Dup) sample preceding the Spike Dup. If one is not found look for the first Analyte sample following the Spike Dup. If no Analyte (or Analyte Dup) can be located an error condition exists (see below).
- If no Spike Dup was located, look for the first Analyte (or Analyte Dup) sample preceding the Spike in the sample list. If one is not found, look for the first Analyte (or Analyte Dup) following the Spike. If no Analyte (or Analyte Dup) can be located an error condition exists (see below).

Errors

- If no Spike sample was located in the rows selected for processing (according to the rules given above), then an error message will be displayed: **Form 3 Error No matrix spike sample identified**
- If no Analyte (or Analyte Dup) sample was located in the rows selected for processing (according to the rules given above), then an error message will be displayed: **Form 3 Error No Unspiked sample identified**

Warnings: If no Spike Dup sample was located in the rows selected for processing (according to the rules given above), then a warning message will be displayed: **Form 3 Warning No matrix spike duplicate sample identified – form will be incomplete.** This is a valid condition, since Spike Dup samples are not always run.

Form 4

Primary data for Form 4 will be taken from a Meth Blank sample with summary information from samples types other than Tune Eval, Init Calib or Cont Calib. The default Meth Blank to be used as the primary data set will be the last Meth Blank sample row selected in the sample list.
Errors: If no Meth Blank sample was located in the rows selected for processing (according to the rules given above), then an error message will be displayed: **Form 4 Error No method blank sample identified**

Warnings: If no rows selected for processing (excluding the Meth Blank row) are of sample type other than Tune Eval, Init Calib or Cont Calib then a warning message will be displayed: **Form 4 Warning Sample list contains no sample types reported in Form 4 summary**

Form 5

Primary data for Form 5 will be taken from a Tune Eval sample with summary information from other samples types (other than Tune Eval). The default Tune Eval to be used as the primary data set will be the last Tune Eval sample row selected in the sample list.

Errors: If no Tune Eval sample was located in the rows selected for processing (according to the rules given above), then an error message will be displayed: **Form 5 Error No tune evaluation sample identified**
Warnings:
If no rows selected for processing are of sample type other than Tune Eval then a warning message will be displayed: **Form 5 Warning Sample list contains no sample types reported in Form 5 summary**
If the Analysis type is Volatiles and the specified Tune Eval file references DFTPP (or Analysis is Semivolatiles and Tune Eval references BFB) then a warning message will be displayed: **Form 5 Warning Tune evaluation sample references the wrong compound for the Analysis type**

Form 6

The data for Form 6 will be taken from the Calibration file referenced by most of the rows in the sample list. The general checks will have ensured that only one Calibration file is referenced. This Calibration file can be taken from any sample row other than the Tune Eval (which is ignored).

The first Analyte (or Analyte Dup) row found in the selected rows of the sample list will be marked as the source of the header information for Form 6. The file name of this sample will be displayed on the Form 6 tab. The user can change this assignment if necessary.

Errors: No errors specific to Form 6.

Warnings: No warnings specific to Form 6.

Form 7

Primary data for Form 7 will be taken from a Cont Calib sample. The default Cont Calib will be the last Cont Calib sample row selected in the sample list.

Errors: If no Cont Calib sample was located in the rows selected for processing (according to the rules given above), then an error message will be displayed: **Form 7 Error No continuing calibration sample identified**

Warnings: No warnings specific to Form 7.

Form 8

Primary data for Form 8 will be taken from a Cont Calib sample (which may be the Mid-Level of an Initial Calibration with summary information from other samples types (other than Tune Eval, Cont Calib or Init Calib types). The default Cont Calib to be used as the primary data set will be determined as follows:

- If the selected sample rows contain Cont Calib rows then the primary data set will be last Cont Calib sample row selected in the sample list.
- If the selected sample rows do not contain a Cont Calib row but contain one or Init Calib rows then the middle row of this set will be marked (in the Status column) as the Cont Calib. If an even number of Init Calib rows are selected then the closest row past the mid–point will be flagged as the Cont Calib. If only one Init Calib row exists then that will be chosen.

Errors: If no Cont Calib sample was located in the rows selected for processing (according to the rules given above), then an error message will be displayed: **Form 8 Error No continuing calibration sample identified**
Warnings: If no rows selected for processing are of sample type other than Tune Eval, Cont Calib or Init Calib then a warning message will be displayed: **Form 8 Warning Sample list contains no sample types reported in Form 8 summary**

Report Method Usage

The following report methods specify templates designed for use from the TurboMass environmental report generation window only. To use these report methods they must be specified in the Submitter/Task Data window's Report Method tab. Examples of these reports in .PDF file format are found in the directories:

C:\TurboMass\Tutorial_VOA.pro
C:\TurboMass\Tutorial_SVOA.pro

IMPORTANT: *Using these report methods in a sample list Report Method column for acquisition or processing could lead to invalid or misleading results.*

Form1TIC_SV	PKI1TIC_SV
Form1TIC_VOA	PKI1TIC_VOA
Form2_SV_soil	PKI2_SV_soil.
Form2_SV_Water	PKI2_SV_water
Form2_VOA_Soil	PKI2_VOA_soil
Form2_VOA_Water	PKI2_VOA_water
Form3_SV_Soil	PKI3_SV_Soil
Form3_SV_Water	PKI3_SV_Water
Form3_VOA_Soil	PKI3_VOA_Soil
Form3_VOA_Water	PKI3_VOA_Water
Form4_SV	PKI4_SV
Form4_VOA	PKI4_VOA
Form5_SV	PKI5_SV
Form5_VOA	PKI5_VOA

The following report methods can be included in a sample list Report Method column to generate reports during acquisition or reprocessing. Where the report method is specific to a particular sample type, the required sample type is indicated in parentheses. Other specific limitations are also indicated in parentheses.

Form1_SV	
Form1_VOA	
Form6_SV	(a valid calibration file must be specified on the sample list row)
Form6_VOA	(a valid calibration file must be specified on the sample list row)
Form7_SV	(Cont Calib samples only)
Form7_VOA	(Cont Calib samples only)
Form8_SV	(report method must appear only on the last row and the first row must be a Cont Calib)
Form8_VOA	(report method must appear only on the last row and the first row must be a Cont Calib)
ICV_SV	(Cont Calib samples only)
ICV_VOA	(Cont Calib samples only)
LCS_SV	(Lab Control samples only)
LCS_VOA	(Lab Control samples only)
PKI1_LCS_SV	Lab Control samples only)
PKI1_LCS_VOA	Lab Control samples only)
PKI6_SV	a valid calibration file must be specified on the sample list row)
PKI6_VOA	a valid calibration file must be specified on the sample list row)
PKI7_SV	Cont Calib samples only)
PKI7_VOA	Cont Calib samples only)
PKI8_SV	report method must appear only on the last row and the first row must be a Cont Calib
PKI8_VOA	report method must appear only on the last row and the first row must be a Cont Calib
PKIEnvQuant	intended for Analyte samples; will give incomplete results for calibration samples)

In addition to the above Report Methods and associated templates, there are three other included templates of use if .CSV (comma separated variable) reports are required. All must be produced within the environmental report generation window. Examples are in the same directories as the .PDF files.

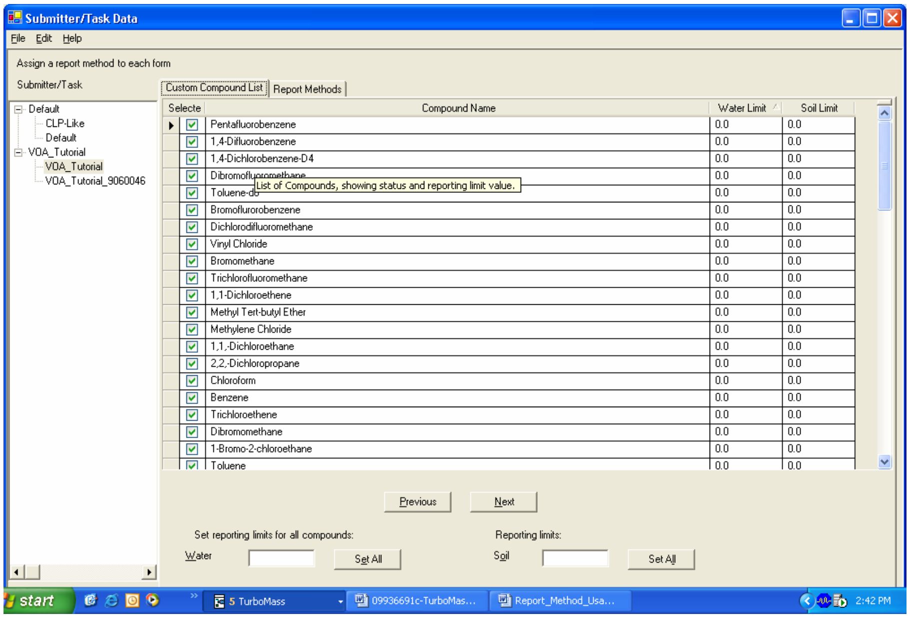
Form1_CSV	(reports both Form 1 and Form 1 TIC)
Form5_CSV	
Form6_CSV	

Submitter/Task Data Window

The Submitter/Task Data Window combines several related functions:

- Maintenance of Submitter/Task hierarchy
- Maintenance of Custom Compound Lists
- Mapping of Forms to Report Methods

These functions are combined in one Submitter/Task Data window since both Custom Compound Lists and mapping of Forms to Report Methods are specific to a Task.



The basic requirements for Custom Compound Lists are that an environmental laboratory should be able to define subsets of the compounds in a quantify method to be reported for a particular project (Task in TurboMass terms) of a particular client (Submitter in TurboMass terms), and also to set the (concentration) reporting level of each of these compounds uniquely for each client's (Submitter's) projects.

The mapping of Forms to Report Methods allows Form customization by providing a translation between the EPA Forms and Communiqué templates (referenced in TurboMass report methods). This translation enables the environmental report generation process, which is driven from the selection by the user of the Forms to be printed, to assemble the appropriate set of report methods/templates automatically.

The Status Bar

When a Custom Compound List is displayed the status bar (located on the bottom of the window) displays the exact origin of the Custom Compound List: the Project name is displayed in the left–hand segment and the Quantify Method name, along with the time and date the compound list was imported, is displayed in the right–hand segment. At all other times the status bar will be left empty.

Submitter/Task List

This window is displayed when the **Submitter/Task Data…** command is chosen from the Environmental Configuration submenu under the Tools menu in the main TurboMass Sample List window. The following Submitter/Task pane on the left side shows a Submitter and Task selected.

This pane is a hierarchical tree view showing clients (Submitters) and their projects (Tasks) displayed in alphabetical order. The tree view can be expanded and collapsed by clicking on the "+" or "-" nodes next to the Submitter names.

Nodes can be renamed by using the right-click context menu.

You can also associate a Custom Compound List with a particular Task, but not directly with a Submitter.

Context Menu for the Submitter/Task List

Right–clicking on a node of the **Submitter/Task** tree view displays the **Context menu**. Note that it will not appear if you click on empty space within the list.

Command	**Description**
New Submitter	Displays the New Submitter dialog to create a new Submitter name.
New Task	Displays the New Task dialog to create a new task for the Submitter.
Collapse All	Closes all expanded nodes so that only the top level nodes are displayed.
Expand All	Displays all nodes.
Rename…	Enables you to change the name of the selected node
Delete	Deletes the Task node and its associated data (compound list and/or report methods)

Info	Displays a Task Info dialog showing the comments entered by the user when the Task was created.

The Submitter/Task Data window has the following Menu item commands.

Menu	**Command**	**Description**
File	Save	Saves the Submitter/Task data.
	Export…	Displays the to export Submitter/Task data from TurboMass to archive or another computer.
	Import…	Displays a File Open dialog, allowing you to select a previously exported Submitter/Task Data file. When a file has been chosen the Import dialog will be displayed.
	Exit	Closes the Submitter/Task Data window. If unsaved changes exist then a dialog will be displayed with the message "Save changes?" and Yes and No buttons. Clicking Yes saves the data. Clicking No closes the dialog and any changes to the data will be lost.
Edit	New Submitter…	Displays the New Submitter dialog to enter a new Submitter. After entering a new submitter Name the OK button will be enabled. Each submitter name must be unique (independent of case). If the entered name is valid, the dialog will close and a new submitter node will added to the tree. If the entered name already exists, an error message is displayed.
	New Task…	Displays the New Task dialog to enter a new task for a submitter.

	Load Compound List…	Displays the Load Compound List dialog. When you have selected a method the compound list is read from the Quantify method and assigned to the selected Task. Initially all compounds are selected for use.
	Select All	Puts a checkmark next to all compounds in the current compound list.
	Unselect All	Removes checkmarks from all compounds in the current compound list.
	Rename…	Allows you to change the name of the selected node.
	Delete	If a Task node is selected, it deletes the task node and its associated data (compound list and/or report methods). If a Submitter node is selected, all Tasks, associated report methods and custom compound lists for this submitter are also deleted. You can recover deleted data by closing the window without saving the data.
Help	Help Topics	Displays the Help topics for this window

New Task Dialog

This dialog displays when **New Task…** is chosen from the Edit menu in the Submitter/Task Data window.

Parameter	Description
Name	An edit box in which you can enter a name of up to 50 characters for the new task. Each task name must be unique for that submitter (independent of case).
Load compound list from Quantify Method	A drop–down list from which you can select the Quantify Method to be used as the source of the compound list.

Browse	Click this button to open a file selector dialog from which you can select a Quantify method from any project.
OK	Each task name must be unique for that submitter (independent of case). If the entered name is valid, the dialog closes and a new task node is added to the tree under the current submitter. If the entered name already exists, an error message will be displayed.
Cancel	Closes the dialog without creating a new task or compound list.

Export Submitter/Task Data Dialog

This Export dialog displays when you select Export… from the File menu in the Submitter/Task Data window. Here you select the Submitters and Tasks with their corresponding Custom Compound List and Report Methods that you want to Export (as a *.CCL file). The default directory is the MethDB directory of your current project.

Parameter	**Description**
Select Submitter/Task data to be exported	Displays the Submitter/Task hierarchy as shown in the Submitter/Task Data window. This includes all of the Submitters and Tasks available with none selected. Click in the box to the left of the item you want to select.
Select All	Clicking this button that will applies check marks to all Submitters and Tasks.
Unselect All	Clicking this button removes any check marks from all Submitters and Tasks.
OK	Clicking this button displays a File Save As dialog allowing you to enter a file name for the exported data and to select the directory where the file will be stored.
Cancel	Clicking this button closes the dialog without exporting any data.

Import Submitter/Task Dialog

The Import dialog displays when you select a previously exported Submitter/Task data file following use of the **Import…** command from the File menu in the Submitter/Task window.

The form of the Import dialog is similar to that of the Export dialog, except for the title and the caption above the tree list are modified appropriately.

Control	Description
Submitter/Task list	Applying a check mark to a Submitter will cause all Tasks belonging to that Submitter to be checked. Unchecking a Submitter will cause all Tasks belonging to that Submitter to be unchecked. Unchecking one or more (but not all) Tasks under a Submitter will cause the Submitter check box to 'gray' indicating there are some Tasks selected and some unselected.
Select All	Clicking this button applies check marks to all Submitters and Tasks.
Unselect All	Clicking this button removes any check marks from all Submitters and Tasks.

OK	Clicking OK imports the selected Submitter/Task data. If a name conflict occurs (i.e., the same Task name already exists for that same Submitter) a dialog displays with the message: Data already exist for Task : <taskname>. Enter new task name. The dialog will include a New name edit box and OK, Cancel and Cancel All buttons. The OK button will be disabled until you enter a new name for the Task. Upon clicking OK the new Task will be created and the data imported.
Cancel	Clicking this button closes the dialog without exporting any data.

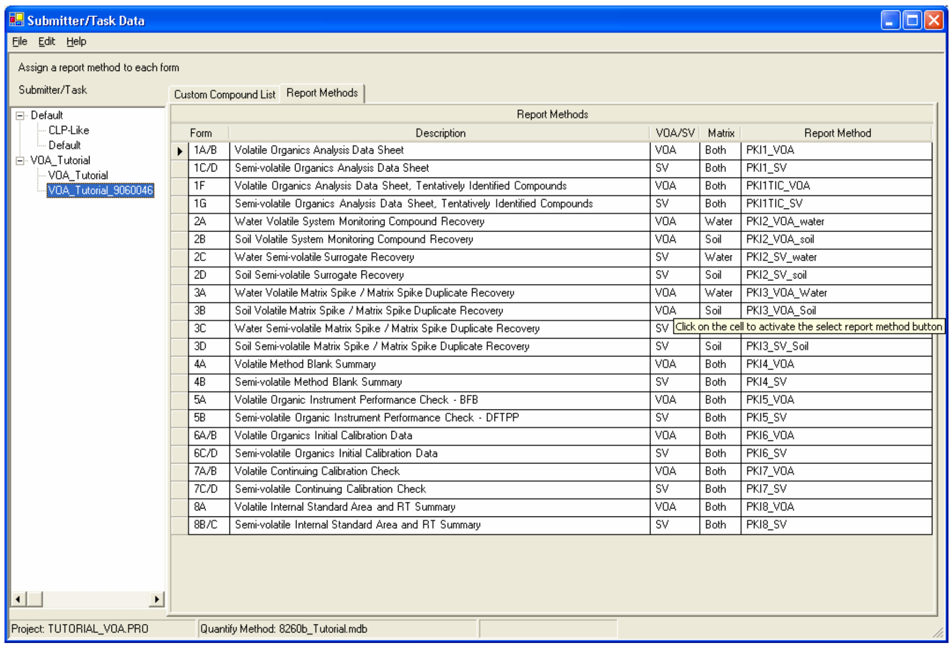
Report Method Tab

An independent mapping of Forms to Communiqué Report Methods can be defined for each Submitter and Task. This mapping is global across all Projects.

NOTE: *It is up to you to ensure the appropriate report methods are in the Project (this occurs automatically when a new project is created via the Project Wizard).*

If specific report methods have not been selected for a given Submitter/Task, then the Default or the most recently selected set will be assigned to that Submitter/Task (see below).

The Report Methods dialog uses the Form descriptions that appear on the EPA Forms. The separate VOA/SV and Matrix columns of the dialog describe when the specific Report Method is used.



In the Report Method form, the only column that contains information that you can change is the Report Method column. The columns can be sized in the standard way by dragging the header divider.

Form	The EPA Form number and subcategory letter (from OLM04.2)
Description	The full description of the Form.
VOA/SV	The analysis type the Form is used for — volatiles or semivolatiles.
Matrix	The matrix type the Form is used for — water samples, soil samples or both.
Report Method	The Communiqué Report Method used to generate this Form. Positioning your cursor in the Report Method column displays a button. Clicking this button displays a file selector for the MethDB directory of the current Project.

To define the report methods

To define the report methods (and hence Communiqué templates) to be used in generating the EPA Forms for an existing Submitter/Task:

1. Choose **Submitter/Task Data…** from the Environmental Configuration submenu under the Tools menu in the Sample List window.
2. Select the appropriate Task for the Submitter.
3. Select the **Report Methods** tab.
4. Review the table displaying Forms 1 to 8, and their variants, together with the associated report method.

5. Where necessary, select the appropriate report method to be associated with each Form. When the mapping of Forms to report methods is correct, choose the **File/Save** command.

Custom Compounds Tab

It is possible to define a subset of the compound list from a Quantify Method and associate it with a Submitter and/or Task name (one list per Task). These subsets can be used for three purposes:

1. During quantitative processing to ensure only the specified compounds are reported and are identified as target compounds for qualitative processing.

2. During qualitative processing to eliminate from the search for Tentatively Identified Compounds only those peaks that are identified as targets for that particularly Task.

The Custom Compound Lists also enable you to define a reporting limit for each compound (i.e., set the “J” flag if the compound is between the Method Detection Limit and the Reporting Limit, or the “U” flag if it is below both) on the Forms.

Once the Custom Compound List has been generated it will retain a reference to the Quantify Method from which it was derived. It is not part of the method and no automatic synchronizing of the custom list with the compound list in the method will take place.

When a **Custom Compound List** is selected the status bar displays the origin of the custom compound list: the Project name is displayed in the left–hand segment and the Quantify Method name is displayed in the center segment.

Item	Description
Compound list	This list shows all the compounds from the selected Quantify Method. Each row has a check box. Checked items will be included in the current Submitter/Task list and unchecked items will be excluded. If the currently selected Task does not have an associated custom compound list then this section of the window is empty. It is possible to sort the compound list in one of two ways: 1. 1. In the order the compounds appeared originally in the main Quantify Method compound list – by clicking on the header of the check box column. 2. In alphabetical (or reverse alphabetical) order – by clicking on the header of the compound name column.
Reporting limits: Water	An edit box that displays the reporting limit value (0.000 to 999,999.999) for water samples associated with the currently selected compound (which may be checked or unchecked). A change made to this field is saved if you click Previous, Modify or Next. If instead you click another compound or another button a dialog displays with the message "Save changes to this compound?" and includes Yes and No buttons. Clicking Yes saves the modified value with the compound. Clicking No leaves the compound's reporting limit unchanged.
Set All	A command button that sets the reporting limit for water samples for all **selected** compounds in the list to the value in the 'Reporting limits: Water edit box.

Reporting limits: Soil	An edit box that displays the reporting limit value (0.000 to 999,999.999) for soil samples associated with the currently selected compound (which may be checked or unchecked). A change made to this field is saved if you click Previous, Modify or Next. If instead you click another compound or another button a dialog displays with the message "Save changes to this compound?" and includes Yes and No buttons. Clicking Yes saves the modified value with the compound. Clicking No leaves the compound's reporting limit unchanged.
Set All	Click this button to set the reporting limit for soil samples for all **selected** compounds in the list to the value in the 'Reporting limits: Soil edit box.
Previous	Click this button to set the reporting limit values of the currently selected compound to the values in the Reporting limits: edit boxes (Water and Soil) and then selects the previous compound in the list.
Modify	Click this button to set the reporting limit values of the currently selected compound to the values in the 'Reporting limits' edit box boxes (Water and Soil).
Next	Click this button to set the reporting limit values of the currently selected compound to the values in the 'Reporting limits' edit box boxes (Water and Soil) and then selects the next compound in the list.

To create a Custom Compound List

To create a Custom Compound List for a new Task of an existing Submitter:

1. Choose **Submitter/Task Data…** from the Environmental Configuration submenu under the Tools menu in the main Sample List window.

2. In the Submitter/Task Data window select the Submitter for whom the new Task is to be generated.

3. Choose New Task from the Edit menu (or the context menu for the tree list), which will display the New Task dialog.

4. Enter a name for the new Task and select the Quantify Method from which the compound list is to be imported. The compounds are displayed and initially each one is checked.

5. Click on the check box to deselect a compound that is not required to be reported for this Submitter/Task. Repeat as required.

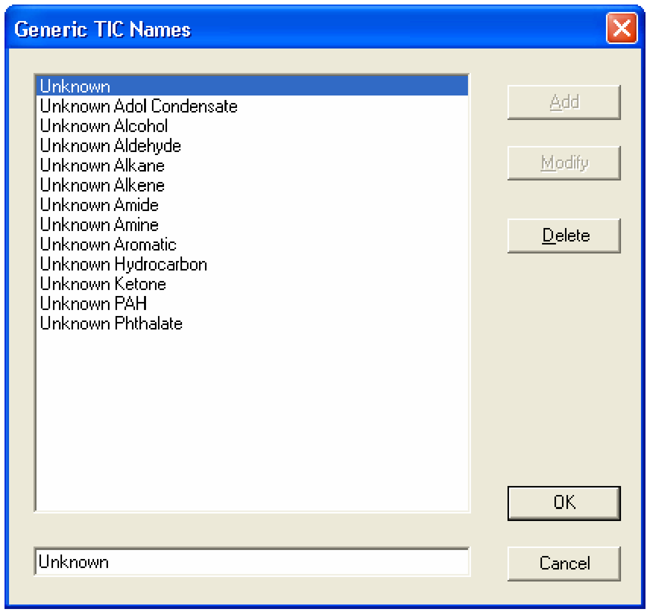
6. Select a compound for which a different reporting limit (Water or Soil) is required. Enter the new value in the appropriate edit field below the list and click **Modify** to save the change or **Next** to save the change and select the next compound (or select Previous to save the change and select the previous compound).

7. Choose **Save** from the File menu to save the new Custom Compound List.

Generic TIC Names Dialog

This dialog enables an administrator (or other person with appropriate access permission) to edit the list of generic compound names that appears in the Tentatively Identified Compounds dialog.

This dialog displays when you choose **Generic TIC Names** from the Environmental Configuration submenu of the Tools menu or clicks the New Name… button in the Form 1 TIC Assign Tentatively Identified Compounds dialog.



Parameter	Description
<list>	A list displaying the currently defined generic names in alphabetical order.
<edit box>	An edit box that enables you to edit an existing name or enter a new name.

Add	Click this button adds the current contents of the edit box to the list as a new entry.
Modify	Click this button to set the currently selected item in the list to the current contents of the edit box.
Delete	Click this button to delete the selected item from the list.

To create/edit a list of generic compound names

To create a list of generic compound names:

1. Choose **Generic TIC Names** from the Environmental Configuration submenu of the Tools menu.
2. Type a generic name into the edit box and click the Add button.
3. Repeat step 2 for each generic name required (the list is sorted alphabetically as each new name is added).
4. Click **OK**

To edit the list of generic names:

1. Choose **Generic TIC Names** from the Environmental Configuration submenu of the Tools menu.
2. Edit an existing name by selecting that name, editing as required and clicking the Modify button.
3. Add a new name by typing the name into the edit box and clicking the Add button.
4. Delete an existing name by selecting the name and clicking the Delete button.
5. Click **OK.**

Appendix A
TurboMass Security

TurboMass Security

The Security application allows a system administrator to control:

- User access to various parts of the TurboMass system.
- Which operations can be performed within a given part of the system.
- Which events are audited.

Security compliments the Windows protection and adds an extra layer of security that is specific to the TurboMass data system.

This appendix defines some security-related terms, provides an overview of the TurboMass security model, and explains how to use the Security Manager to configure user accounts, user groups, and how to assign group privileges.

Security Terminology

This section defines the security terms used in this appendix.

Access Rights/Privileges

By controlling access rights or privileges, administrators can control or restrict the actions of a group of users. Access rights are assigned to groups, and users are members of groups. Access rights cannot be assigned directly to individual users. Users have the access rights assigned to the group(s) to which they belong. Only users who are members of groups with the Administer User Accounts and Groups access right can assign rights to other groups.

Administrator

The administrator is the person responsible for managing the system, adding and removing users and groups, and assigning access rights. The administrator has unlimited access to TurboMass and to the Security application. The Administrator account is always present, with full access, and only the password can be changed. This account cannot be deleted. Administrative privileges can be granted to any user by placing that user in the Administrators group.

Audit Log

The audit log file contains a historical list of events showing which users accessed or attempted to access objects covered by the list of access rights. Auditing can be customized so that only certain categories of event are included, or disabled completely. An audit log viewer is provided within the Security Manager.

Group

A group is a collection of TurboMass users. A group can have access rights assigned to it to restrict their movements within the data system. Groups provide a convenient way of managing the capabilities of users (it is often easier to remember which privileges a particular group has, rather than those of an individual). The Administrators group cannot be deleted and always has full access rights.

Group Rights

See *Access Rights/Privileges*.

Logon Name

The logon name is the name by which a user is known to Security. Each logon name has an associated password and user account. To log in to Security, a user must provide a valid logon name and password.

Password

A specific word used to log on when Security is enabled that verifies the user's identity. Passwords are case-sensitive.

Right/Privilege

See *Access Rights/Privileges*.

Security Manager

The TurboMass application that administers the TurboMass security system. The Security Manager cannot be run at the same time as TurboMass.

User

A TurboMass user who usually has more limited access privileges than an Administrator.

User Account

A record maintained by Security that contains information about a particular user.

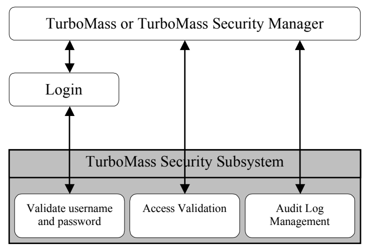
Username

The name by which a user is known to TurboMass. A user logs on to TurboMass by providing a valid username and password. A user's group rights determine his individual rights.

Security Model

The Security Model is based on user accounts. Users are members of groups, and groups have access privileges. A user cannot be directly given an access privilege.

The Security system performs tasks such as user account management, group management and audit log maintenance, and logs users in and out and verifies their access privileges.



Validate Username and Password

The system within Security that verifies a username and password TurboMass against the existing user accounts. If Security finds an account for the specified username and the password is correct, the user is allowed to proceed. All subsequent access requests can then be validated. Any information written to the audit log contains a reference to the username.

Access Validation

When a user attempts to enter a TurboMass or a Security Manager-protected area, the Access Validation subsystem determines the access rights of the groups to which the user belongs. An entry is also written to the audit log to reflect the outcome of the access attempt.

Audit Log Management

The audit log management system maintains the audit log.

Security Manager

The Security Manager is used by an administrator to assign access privileges and set up user accounts and groups.

Specifically, an administrator can perform the following tasks:

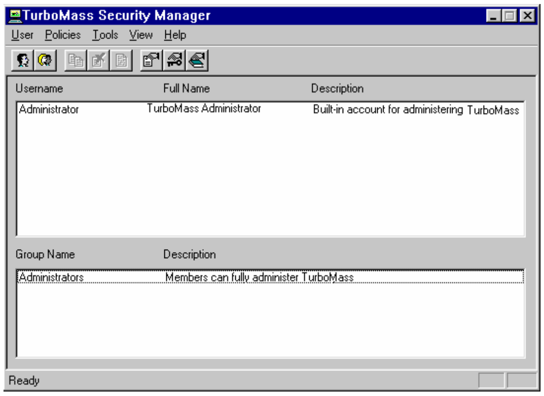
- Create, delete, and edit user accounts.
- Create, delete, and edit groups.
- Assign access privileges to groups (Group rights policy).
- Set the account policy.
- Disable Security.
- Set the audit policy.
- View and manage the audit log.

NOTE: *TurboMass Security and TurboMass cannot be run simultaneously. Close TurboMass before opening the Security application.*

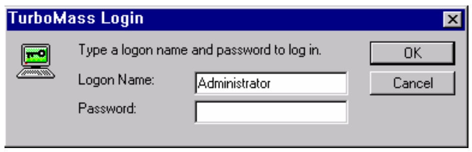
If Security is enabled when TurboMass is opened, the user is required to log on to TurboMass by entering a username and password into the Login dialog.

Logging on to TurboMass with Security enabled

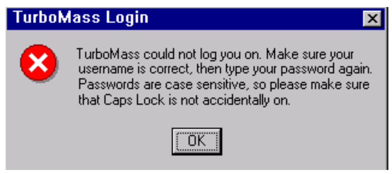
1. Double-click the Security icon in the TurboMass program group to open the Security Manager dialog.



If security is enabled, TurboMass displays the Login dialog.



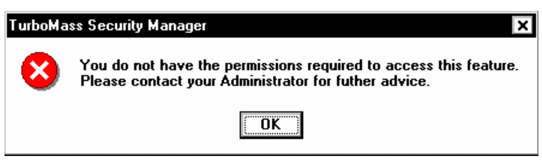
2. If the following message is displayed, verify the password and username.



3. If the message remains, verify that the user has a valid account with Security.

   Make sure that the account has not been disabled.

   The username determines the user's level of access allowed within TurboMass or the Security Manager. If the user does not have full administrative privileges, the following message may be displayed:



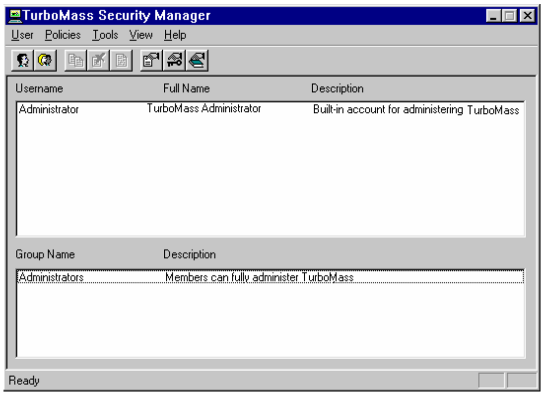
4. If a user needs access to a particular area, assign the user to a group that has the necessary access privileges. See Assigning an access privilege to an individual user on page 676 for more information.

   If the username entered does not belong to a group with administrative privileges, the user is limited to viewing their own account information.

Changing a password without administrative privileges

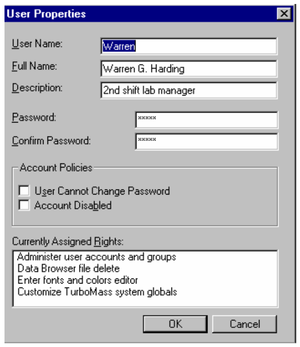
1. Exit TurboMass, if necessary.

2. Start the Security application to open the Security Manager dialog and display a list of user accounts.



3. Select the account for which you want to change the password, and select **Properties** from the **User** menu.

   The User Properties dialog is displayed.



4. If the Password fields are available, enter and confirm the new password.

5. If the Password fields are unavailable, administrative privileges are required to change the password for the selected account.

Security Manager Toolbar

The toolbar displayed at the top of the Security Manager dialog contains the tool buttons listed below. The tool button functions are duplicated in the Security menus.

 Creates a new user.

 Creates a new group.

 Copies the currently selected group or user account.

 Deletes the currently selected group or user account.

 Edits the currently selected group account or user properties.

 Reviews the user account policy options.

 Reviews the group access rights.

 Reviews the audit policy options.

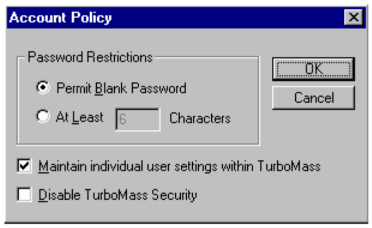
Setting up an Account Policy

Before you create a user account or group, you must specify an account policy to establish the password restrictions and the policy for individual user settings. You can also enable or disable the TurboMass Security application.

1. Select Account from the Policies menu

   Or

   Click  to display the Account Policy dialog.



2. Specify account policy by editing the following parameters:

Permit Blank Password	Creates or modifies a user account to have no password.
At Least X Characters	Specifies the minimum number of characters that passwords must contain. This parameter applies to new user accounts, or to modified user accounts.
Maintain individual user settings within TurboMass	Allows TurboMass to maintain its settings (parameter values, window positions) on a per-user basis. If this option is not selected, any changes made within TurboMass affect all users.
Disable TurboMass Security	Disables the Security application. If Security is disabled, no login prompt is displayed, and all users are logged on with the Administrator

username and with full administrative privileges.
In order to disable Security, you must have administrative privileges, and you must exit TurboMass.

Creating a User Account

There are two ways to create a user account:

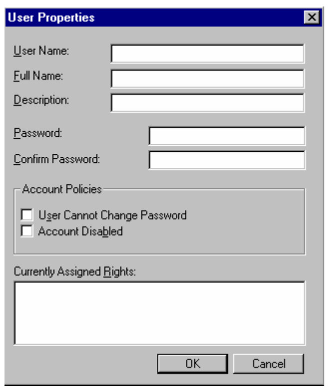
- Enter the new user information into a new user account.
- Copy an exiting user account, edit the policy options, and save the account under a new user name.

Creating a user account

1. Select New User from the User menu

   OR

   Click  to open the User Properties dialog.



2. Enter the new user information.

User Name	The name that a user enters to log on to TurboMass.
Full Name	The user's full name.
Description	A brief user description, for example, position in the company.
Password	A user's default password, which a user can later change (unless **User Cannot Change Password** is selected).
Confirm Password	The user must correctly re-enter the default password to confirm it.
User Cannot Change Password	If selected, the user is not allowed to change their own password.
Account Disabled	Disables the account. When selected, the account's user name cannot be used to log on to TurboMass, but the account information remains intact.
Currently Assigned Rights	The 1ist of rights that is granted to the current user. This list depends on the rights that are assigned to the groups to which the user belongs. When creating a new user (or copying an existing user), this list is empty and unavailable.

NOTE: *A system administrator can change a user's password at any time.*

3. Click OK.

   Security adds the new user to the list, unless the name already exists in the list of users or groups, or the password is too short. See *Setting up an Account Policy* on page 669.

OR

1. Select an existing user from the list in the Security Manager dialog.

2. Select **Copy** from the **User** menu to open the User Properties dialog, and enter the new user information.

Security creates a new user with some of the User Properties information already entered. Until assigned new rights, the new user is a member of the same groups as the original user.

Creating a Group

When you create a user group, the individual members have those access rights granted to the group. You can create a new group by adding members as desired, or you can copy an existing group. Once you have created a group, you will assign access rights to the group.

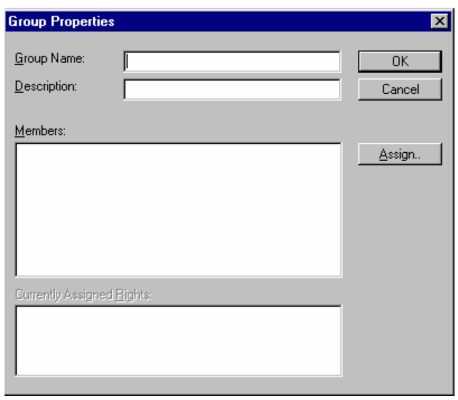
Creating a group

1. Create a new group by doing one of the following:

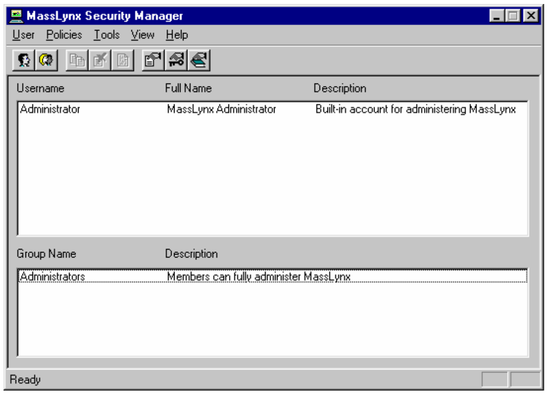
- Click 

  OR

  Select **New Group** from the **User** menu to open the Group Properties dialog.



- Select an existing group from the list in the Security Manager window, and select **Copy** from the **User** menu to copy the existing group.

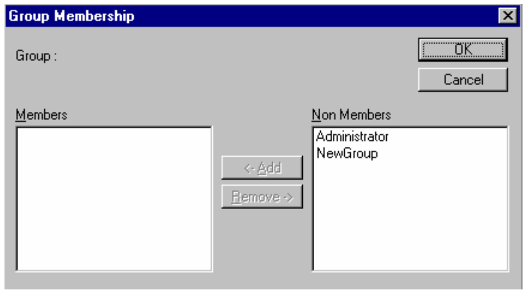


When you copy an existing group, the Group Properties dialog contains some of the information from the copied group, and the new group inherits all the members and group rights from the copied group.

2. Enter the new group information:

Group Name	The name assigned to a group of users.
Description	A brief description of the group, for example, department, or tasks performed.
Members	The list of users who belong to a group. The **Members** list is empty when you are creating a new group. If you create a new group by copying an existing group, then Security copies the list of members from the original group to the new group.
Currently Assigned Rights	The list of rights granted to the current group. When creating a new group (or copying an existing group), the list is empty and unavailable.

3. For each member you want to add, click **Assign** to open the Group Membership dialog, select the user you want to add from the **Non Members** list, and click **Add** to move the new member to the **Members** list.



4. For each user you want to remove, select the user you want to remove from the **Members** list, and click **Remove** to move the selected user from the **Members** to the **Non Members** list.

5. Click **OK** to return to the Group Properties dialog.

6. Click **OK** to return to the Security Manager window.

   The new group name appears in the list of groups.

Deleting a user account or group

1. To delete a user account or group, select the user or group from the relevant list in the Security Manager dialog, and select **Delete** from the **User** menu.

2. Click **OK** to confirm the deletion.

   Security removes all traces of the user account or group. If you create a subsequent user or group with the same name, TurboMass treats it as a new user account or group. For example, you will need to set up group rights and group membership for the new group.

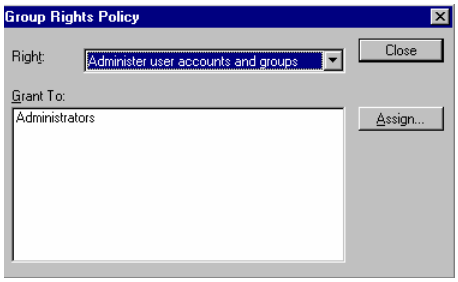
NOTE: *The Administrator user account and the Administrators group cannot be deleted.*

Assigning group rights

1. Select **Group Rights** from the **Policies** menu

   OR

Click  to open the Group Rights Policy dialog.

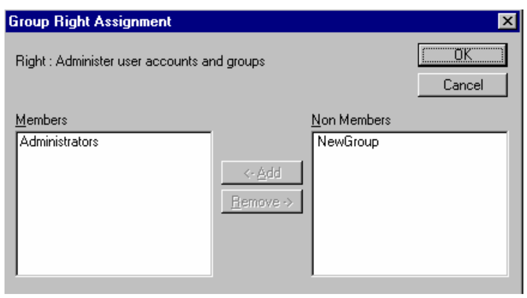


The dialog lists the group(s) that have access to the currently selected right.

Right	A group of access privileges that can be granted to groups. The Administer User Accounts and Groups right refers to the various tasks performed within the Security Manager, any group granted this privilege can modify user accounts and groups, and perform policy changes (such as changing group rights). This right should only be assigned to groups that require administrative privileges.
Grant To	The list of groups that have the currently selected right.

2. From the **Right** drop-down list, select the right you want to assign to the group.

3. To grant the selected right to a new group, click **Assign** to open the Group Right Assignment dialog, select the group in the **Non Members** list, and click **Add** to move the new group to the **Members** list.



Security moves the selected group to the **Members** list.

Repeat step 3 for each group to be granted a new access right.

4. To remove a group from the **Members** list, select the group you want to remove, and click **Remove** to move the selected group to the **Non Members** list.

   The Administrators group cannot be removed from the **Members** list of any group because administrators must have full access rights.

Assigning an access privilege to an individual user

1. Follow the procedure *Creating a Group* on page 672 to create a special group for the user, and make the user a member of the new group.

2. Assign the access privilege to that group using the procedure *Assigning group rights* on page 674.

Managing the Audit Log

The audit log maintains an audit trail of the TurboMass use by tracking each occurrence of each auditable event specified in the Audit Policy. You can set up the Security Audit policy from the Audit Policy dialog. You can monitor the audit log from the Audit Log Viewer.

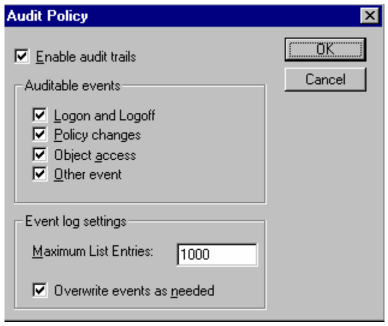
Setting up an audit policy

1. From the Security Manager window, click 

   OR

   Select **Audit** from the **Policies** menu.

   The Audit Policy dialog is displayed.



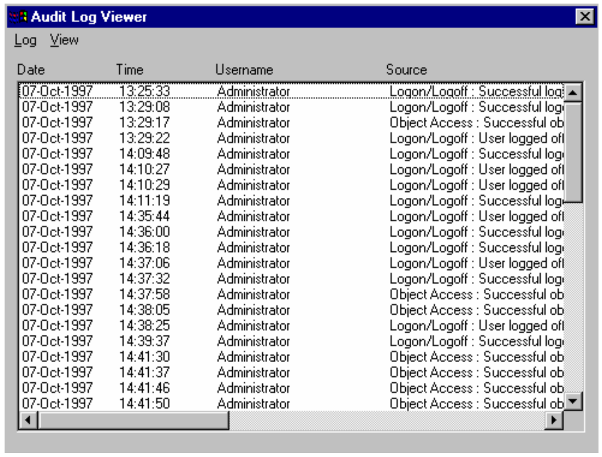
2. Select the auditable events that you want to monitor in the audit log, and specify the event log settings.

Enable audit trails	When selected, audit information is written to the audit log. Deselecting this checkbox disables the audit log, and the audit log is not updated when an auditable event occurs.
Auditable events	The auditable events checkboxes determine which event types are written to the audit log file.
Maximum List Entries	Use this field to specify the maximum number of entries allowed in the audit log. After the specified number of entries is reached, the **Overwrite events as needed** setting automatically takes effect.
Overwrite events as needed	If selected and the number of list entries exceeds the **Maximum List Entries** specified, then Security replaces older entries with newer ones, as necessary. If not selected, new entries are not added after the **Maximum List Entries** value is reached.

Monitoring audit log

1. From the Security Manager window, select **Audit Log Viewer** from the **Tools** menu.

The Audit Log Viewer dialog is displayed.



The Audit Log Viewer displays the audit log that lists the date and time of each auditable event. The **Source** column shows the type and a brief description of each event.

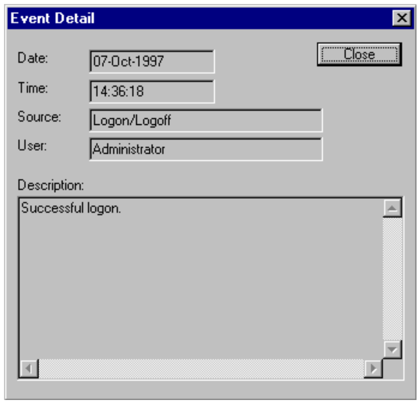
2. Manage the audit log from the Audit Log Viewer dialog Log and View menus:

Log

Clear All Events	Select to completely clear the audit log. Do this periodically because a very large audit log may slow TurboMass processing.

View

Newest First	When selected, displays the most recent event first.
Oldest First	When selected, displays the events in order of occurrence - the first event in the list is the oldest.
Detail	Displays detailed information about a selected Audit Log entry.



Refresh Reopens the Audit Log.

Appendix B TurboMass Software Installation

TurboMass Software Installation

NOTE: *The computer must have Windows XP with Service Pack 2 installed as the operating system.*

The TurboMass software is preloaded on your system by your Service Engineer; however, there may be a time when you need to reinstall the software or upgrade from a previous version. This procedure describes how to upgrade or reinstall the TurboMass software. If you have any questions, or you need to re-configure the Ethernet communications to the mass spectrometer, please contact your local PerkinElmer Service Representative.

During the installation you will be prompted to do the following:

- Confirm the installation directory.
- Confirm your setup options.
- Confirm your instrument pre-configuration options.

IMPORTANT:

Before installing TurboMass v5.2, first ***uninstall the existing TurboMass, Communiqué, and MATLAB*** *using the Add/Remove Programs function in the Windows XP Control Panel.*

When installing TurboMass v5.2, it will automatically detect a Communiqué 1.x database from TurboMass v5.0 and export those templates to c:\turbomass\c1ExportedTemplates directory. After installing v5.2 you can go to that directory and import the templates. Upgrading from TurboMass v5.1 will save a backup copy of your templates database.

We strongly recommend that you manually export all user-modified templates from TurboMass to your hard drive using the Communiqué Utilities or the Communiqué Report Creator (Template Designer), before uninstalling TurboMass v5.0 or v5.1.

After installing TurboMass v5.2 use the Communiqué Utilities or the Communiqué Report Creator to Import the templates into v5.2. All v5.0 and v5.1 TurboMass templates have been updated in v5.2, so do not import your modified templates using the same names.

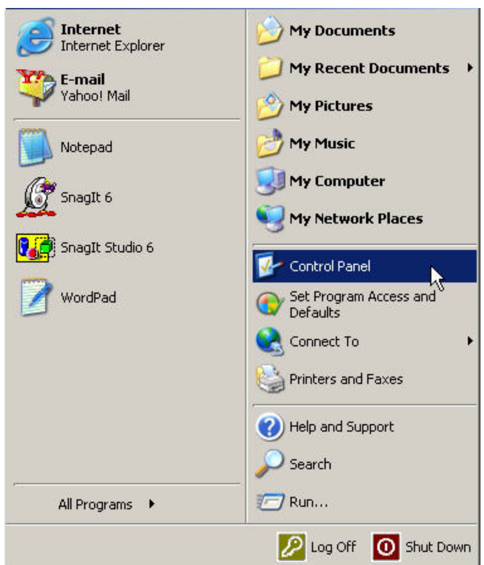
After installing the software and rebooting the computer ***cool the transfer line*** *and ion source to below 100 °C, then* ***you must turn the MS power off then back on again*** *(after at least 5 seconds) to ensure correct installation of the updated software into the instrument.*

Installation Summary

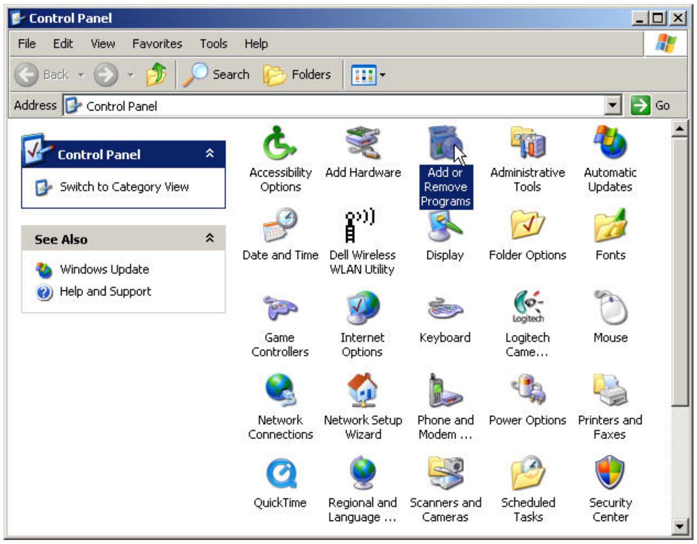
1. Uninstall the TurboMass 5.X software and all its components.
2. Install the TurboMass v5.2 software.
3. Reboot the Clarus MS.
4. Install Clarus 500 MS NIST/EPA/NIH Library (2002)
5. Configure TurboMass for GC control.

Uninstalling the TurboMass Software and all of its Components

1. From the Windows XP desk top click on **Control Panel**.

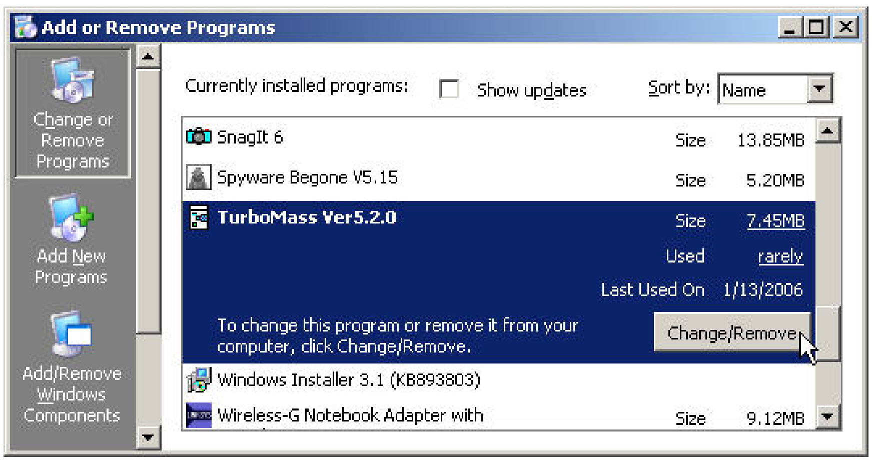


The **Control Panel** dialog appears:



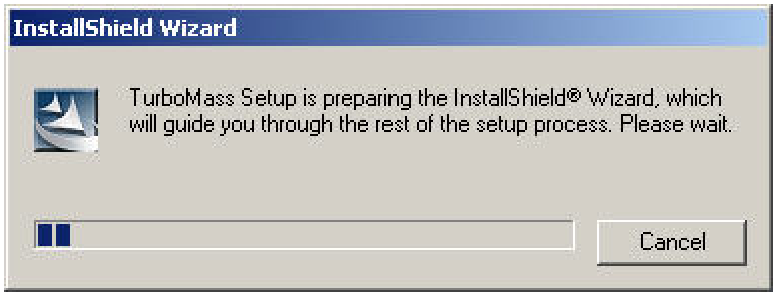
2. Click on **Add or Remove Programs**.

   The Add or Remove Progeams dialog appears:



3. On the Add or Remove Programs dialog select **TurboMass Ver5.X** and click on **Change\Remove.**

   The Uninstall shield loads. Do not click **Cancel** unless you want to halt the unistallation**.**

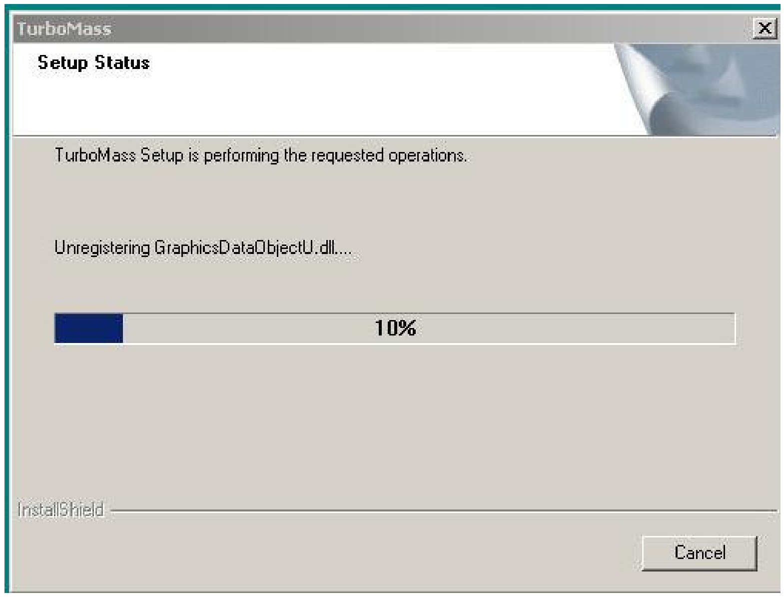


The following appears:

4. Click on **OK** to start the software removal.
   The following appears:

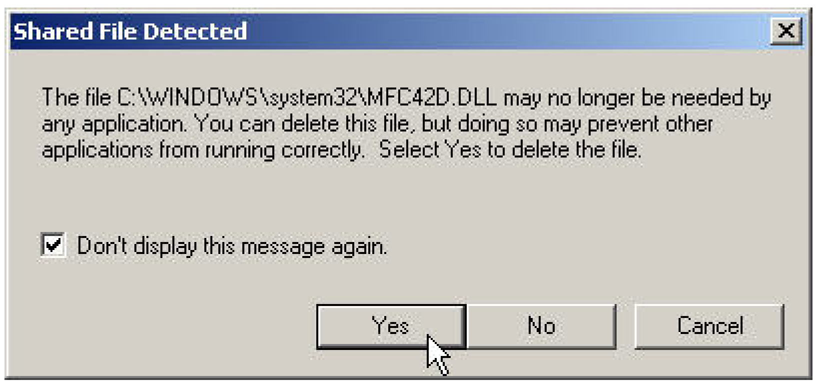
5. Click on **OK** a second time to confirm.
   The following appears:

Then, the LCD Stops if running and the following appears:

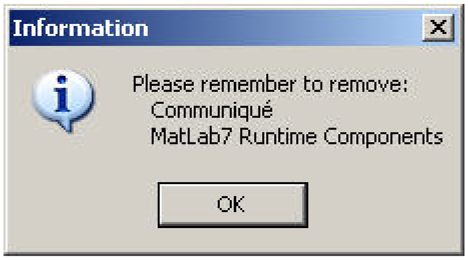


Uninstall continues (this may take several min).

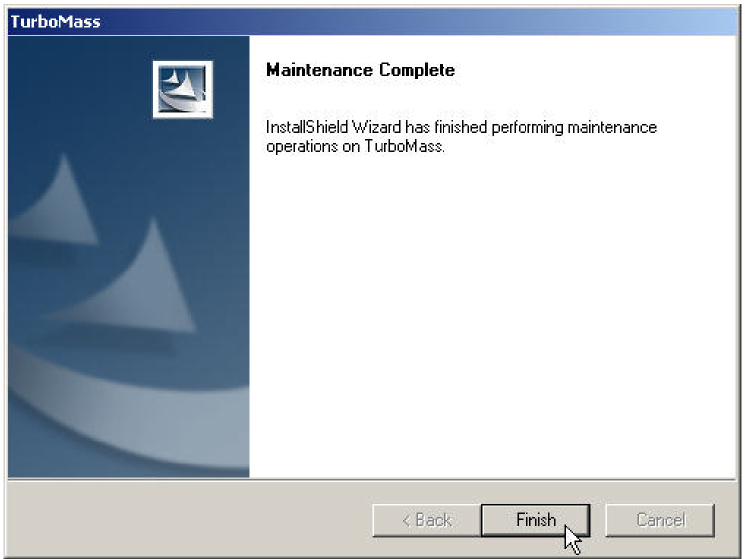
The following appears:



6. (Click the check Box) and Click on **Yes.**
   The following appears:

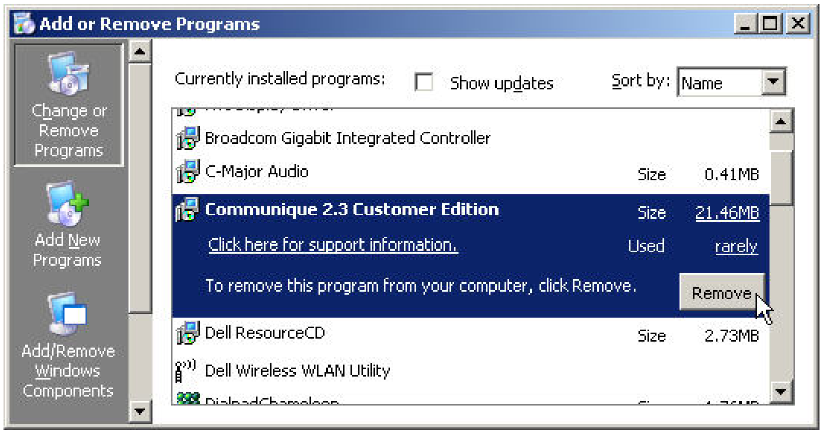


7. Click on **OK.**
   The following appears:

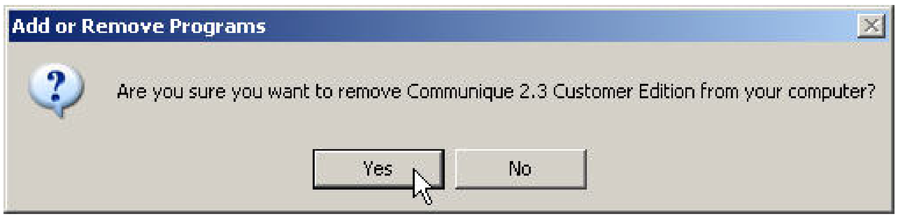


8. Click on **Finish.**

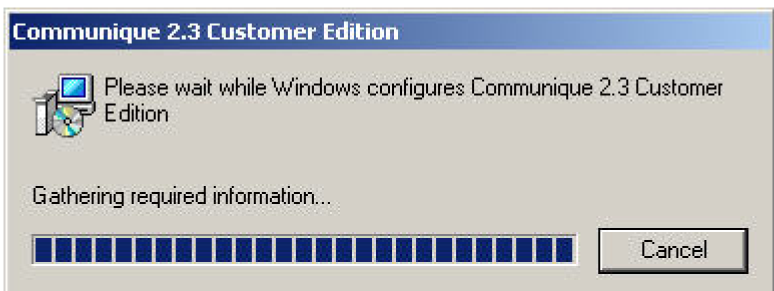
9. On the Add or Remove Programs dialog select ***Communiqué*** **2.3 Customer Edition** and click on **Remove.**



The following appears:

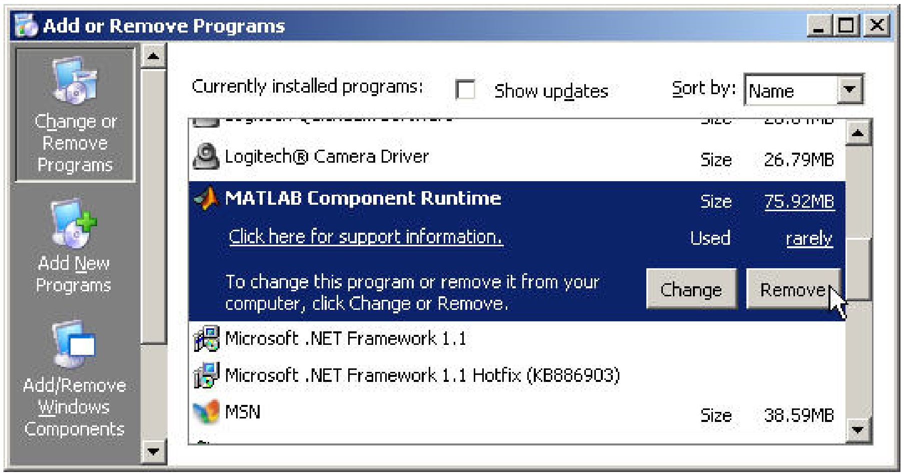


10. Click on **Yes**.
    The following appears:

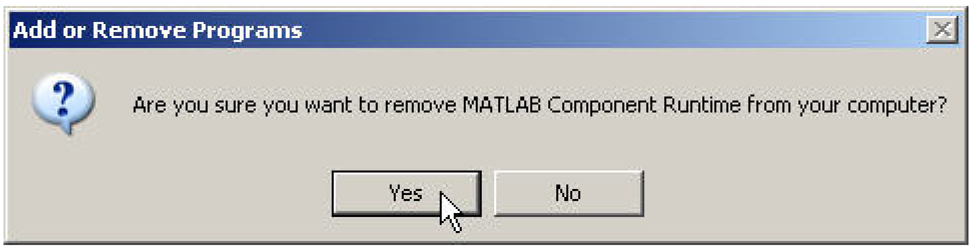


Uninstall runs when complete uninstall MatLab.

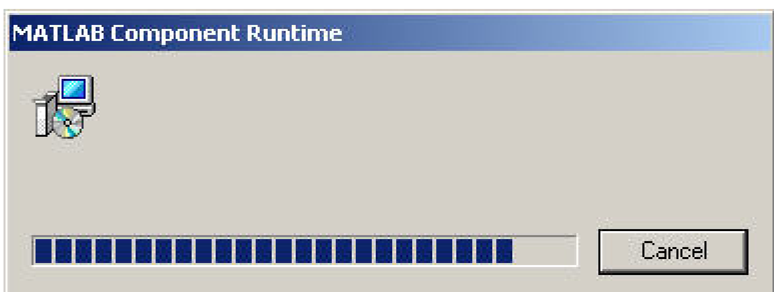
11. On the Add or Remove Programs dialog select **MATLAB Component Runtime** and click on **Remove.**



The following appears:

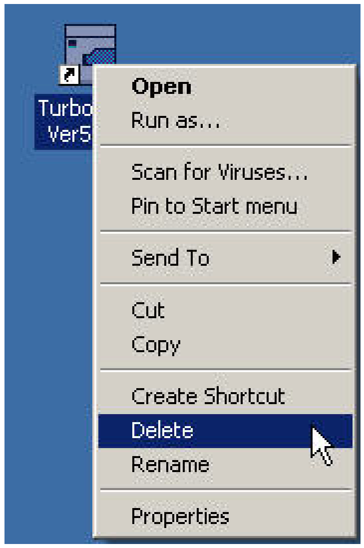


12. Click on **Yes.**
    The following appears:



MATLAB is removed.

13. Delete the Desktop icon.



14. Reboot the computer.

Installing the TurboMass software

1. Verify that all pre-installation tasks are done. See the IMPORTANT information on the first page of this section.

2. Save all data and close all Windows programs.

3. Insert the TurboMass compact disk in the CD-ROM drive.

   The installation program automatically starts and guides you through the installation process with a series of dialogs that prompt you for your choices. The following three buttons are always displayed at the bottom of each setup dialog:

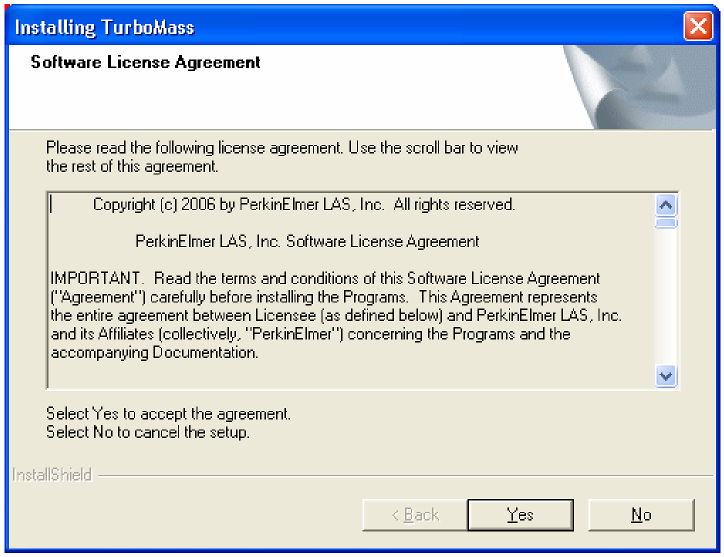
   - **Back** — Go to the previous screen.
   - **Next** — Go to the next screen.

     Click this button when you have completed a dialog.
   - **Cancel** — Stop the installation process and quit the setup program.

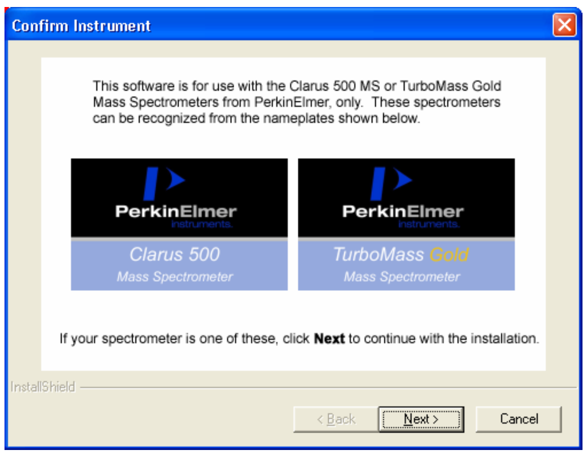
   The rest of this procedure describes the TurboMass installation process and shows the corresponding screens.

   The installation process begins automatically with the Software Licence Agreement.

4. Click **Yes** to accept the agreement or click No to cancel the setup procedure.

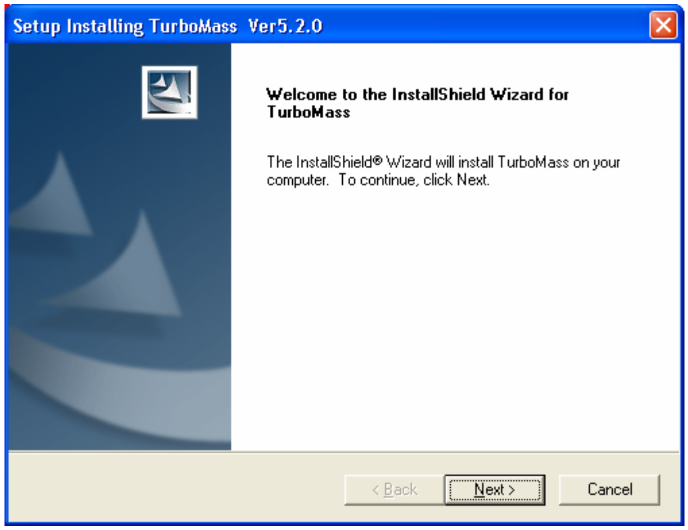


After clicking Yes the **Confirm Instrument** dialog displays. Verify that the software will work with one of these two mass spectrometers.



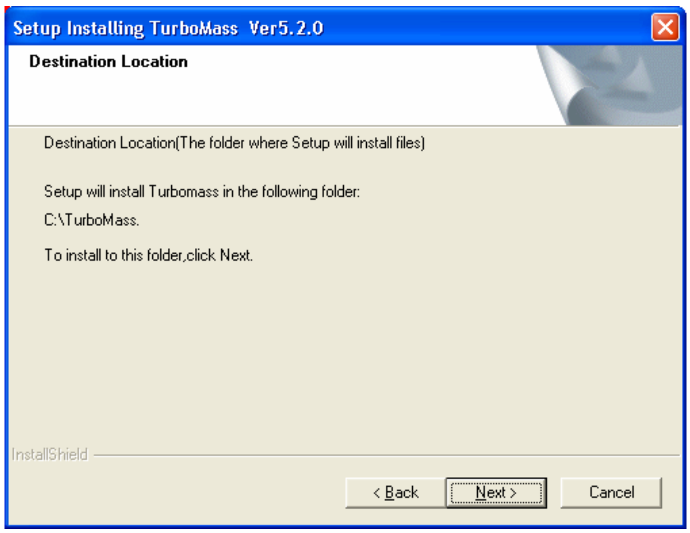
5. Click **Next** to proceed with the installation.

   The Install Shield Welcome dialog displays:



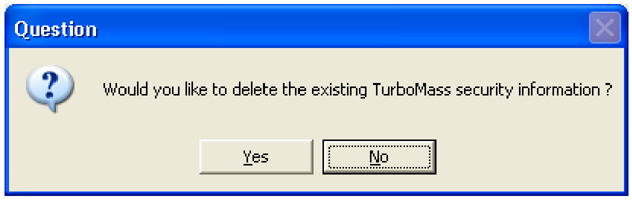
6. Click **Next.**

   The **Destination Location** screen appears.

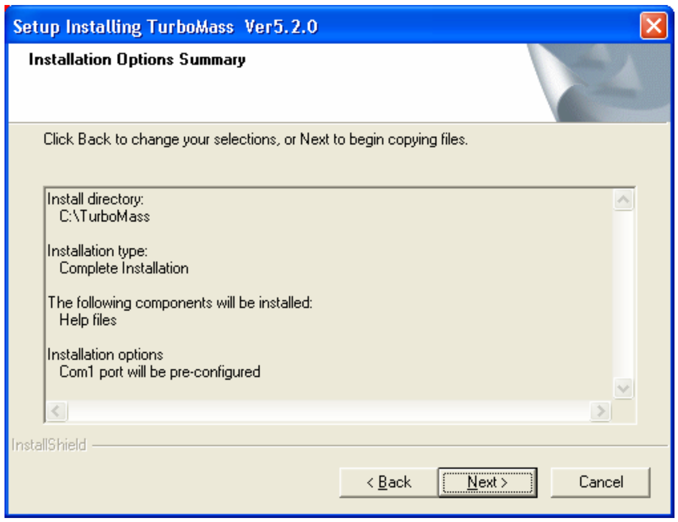


7. Accept the default directory by clicking **Next.**

If TurboMass software had previously been installed, the install wizard next prompts to delete any existing security information. Click **Yes** to continue and delet any previous password information. Clicking **No** will save any previous password.

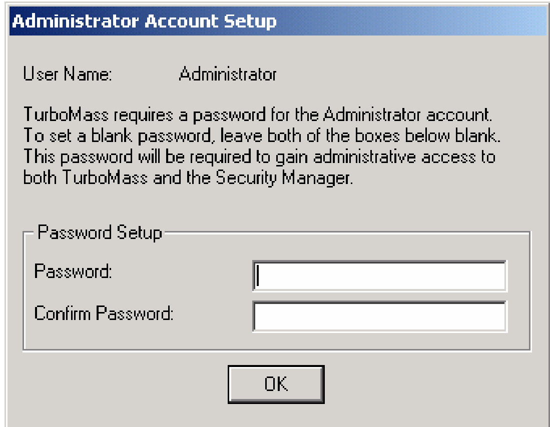


The **Installation Options Summary** dialog opens. This dialog allows you to review your setup choices before the installation process begins.



8. Click **Next** to continue the installation.

   The Administrator Account Setup dialog appears:

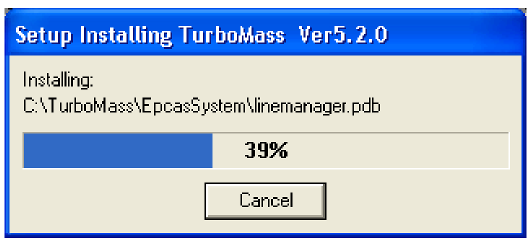


You can either create a password here or leave both boxes blank for no password.

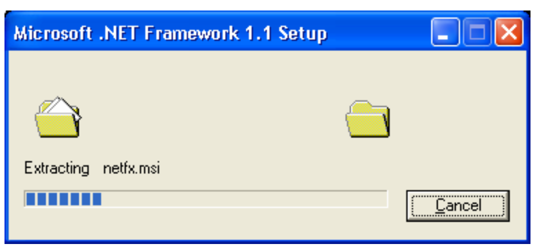
NOTE: *If the password is forgotten, the software will have to be reinstalled!* ***Remember your password***.

9. Click **OK** to continue the installation.

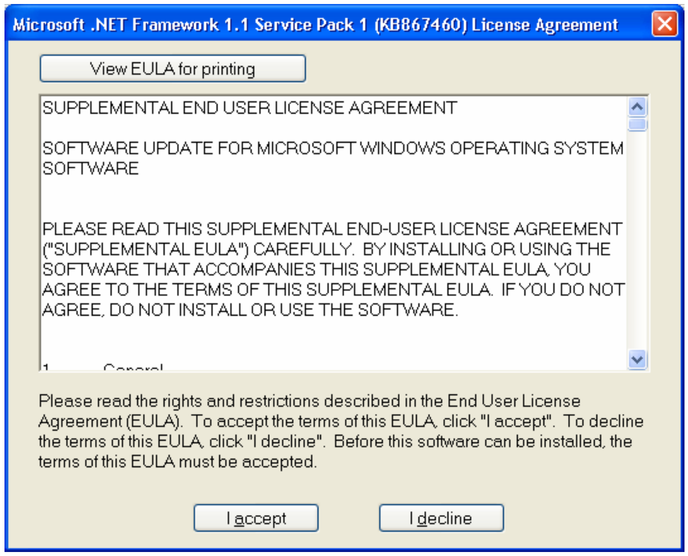
   TurboMass starts installing.



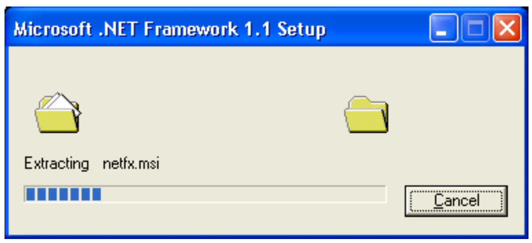
10. The .NET Framework also starts to setup.



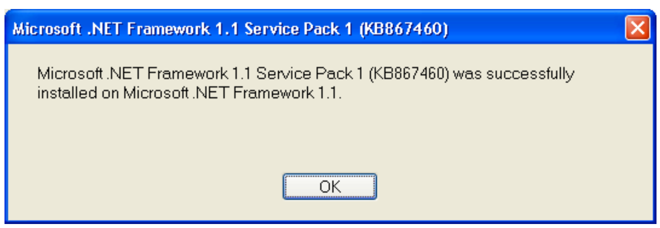
11. Click **OK** and the following appears:



12. Click **I accept** to start installing the .NET Framework.

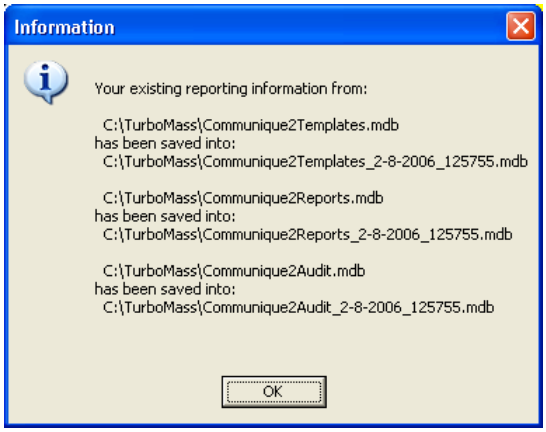


When complete the following appears:

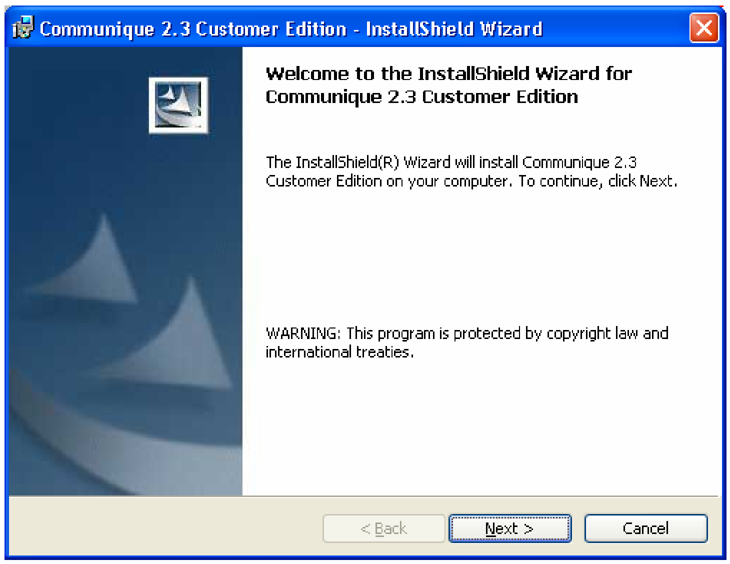


13. Click **OK**.

If any Communique Reporting templates had been stored from a previous version of TurboMass software, the following dialog appears verifying they have been saved:

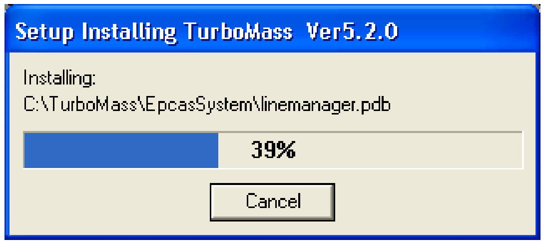


14. Click **OK** and the **Welcome to the Install Shield Wizard for Communiqué** appears:

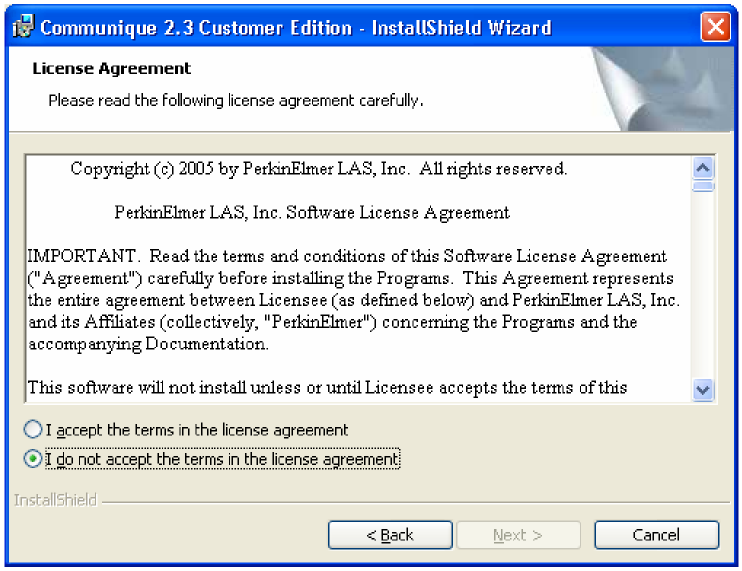


15. Click **Next** to continue the installation.

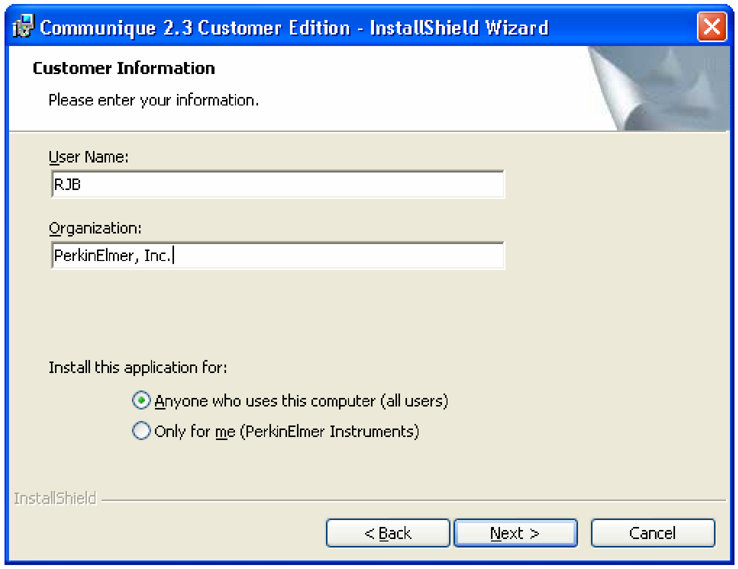
 The following message appears:



The Communique License Agreement appears:



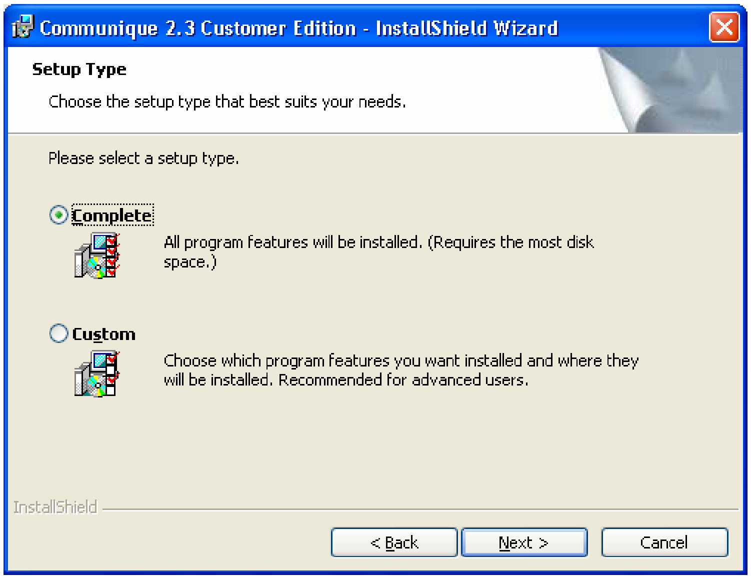
After accepting the terms of the license agreement, click **Next. The Customer Information** dialog appears:



Select the option "**Anyone who uses this computer (all users)**".

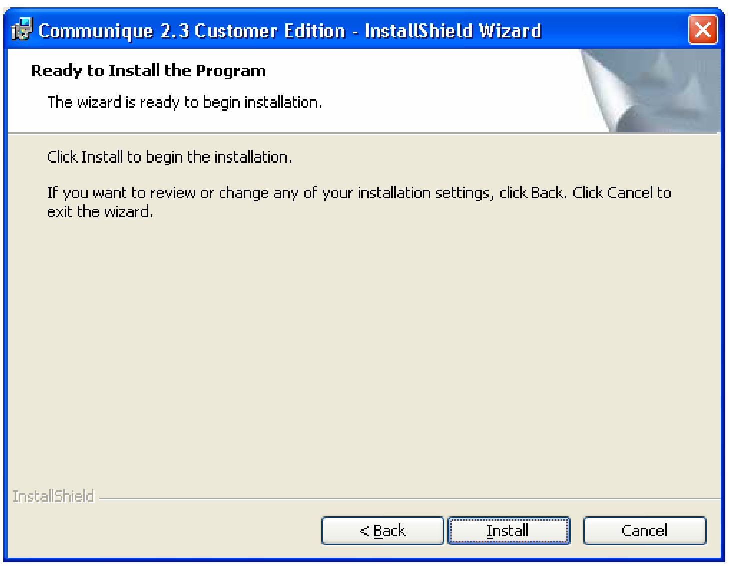
16. Enter the requested information and click **Next** to continue the installation.

    The **Setup Type** dialog appears:



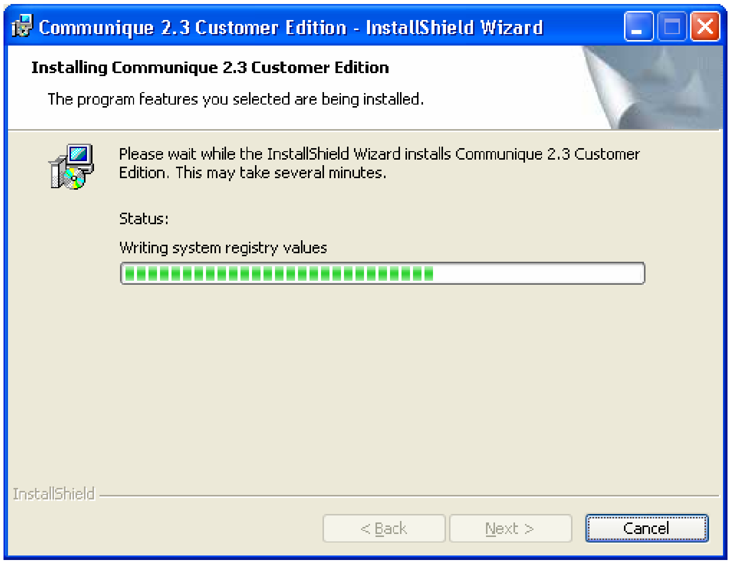
17. Select **Complete** and click **Next**.

    The **Ready to Install the Program** dialog appears:

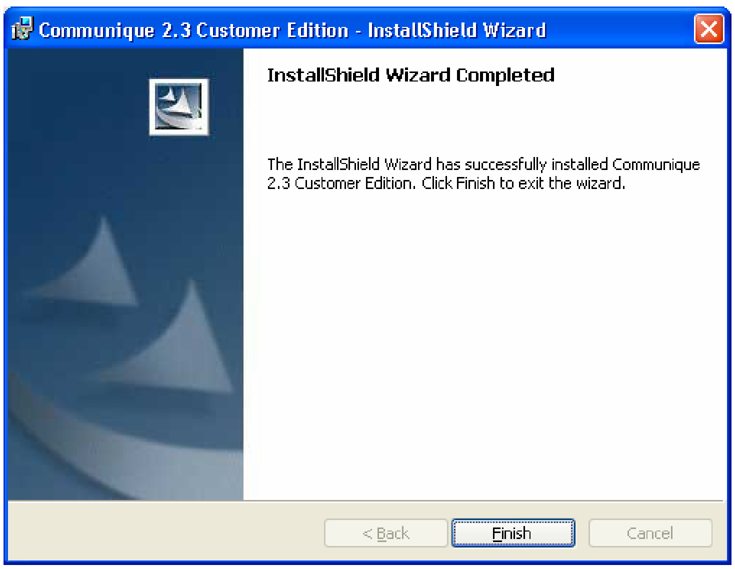


18. Click **Install** to continue the installation.

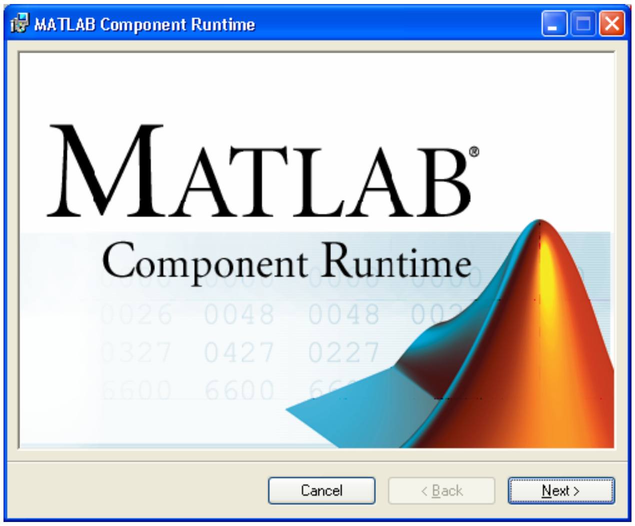
    Communique installation begins.



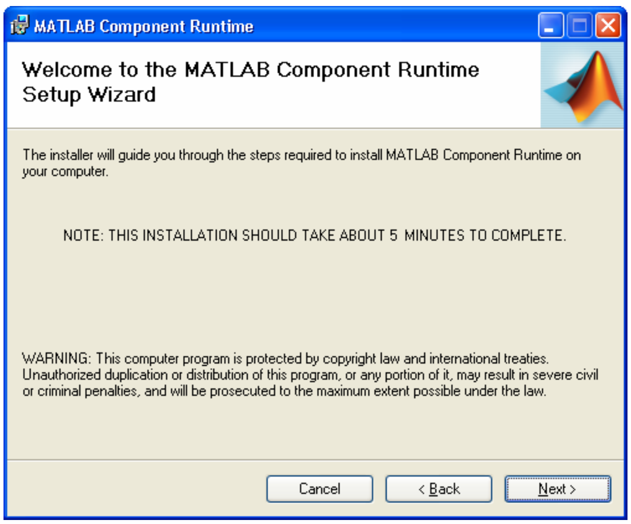
The install process continues until the Install Wizard Complete screen is displayed.



19. When complete, click **Finish** and start the MATLAB installation.
    The MATLAB screen appears:



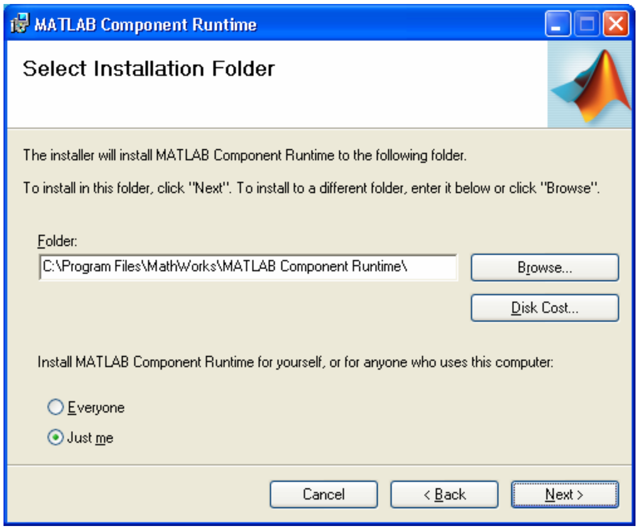
20. Click **Next** to continue with the installation.



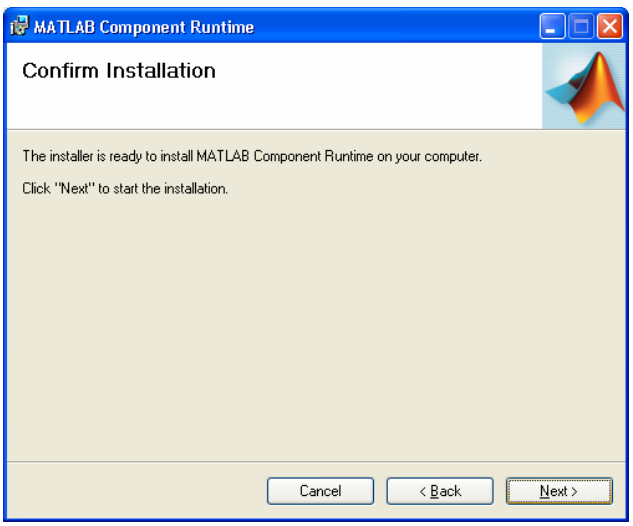
21. Click **Next** to continue. The **Select Installation Folder** dialog appears:

NOTE: *Do not change the folder path. MATLAB components only work when MATLAB is installed in the default path.*

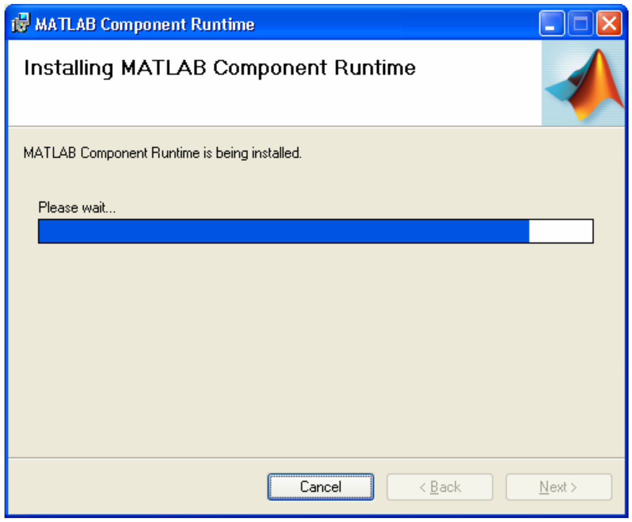
NOTE: *The default install for MATLAB specifies "Just Me". Change the default setting to* **Everyone** *and click **Next** to continue.*



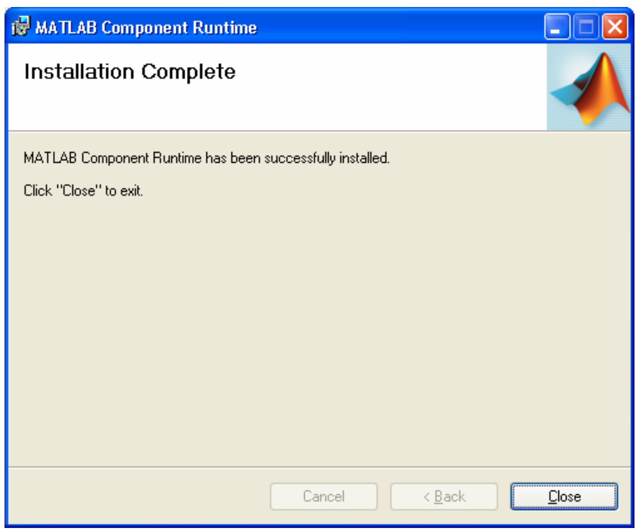
The following dialog appears:



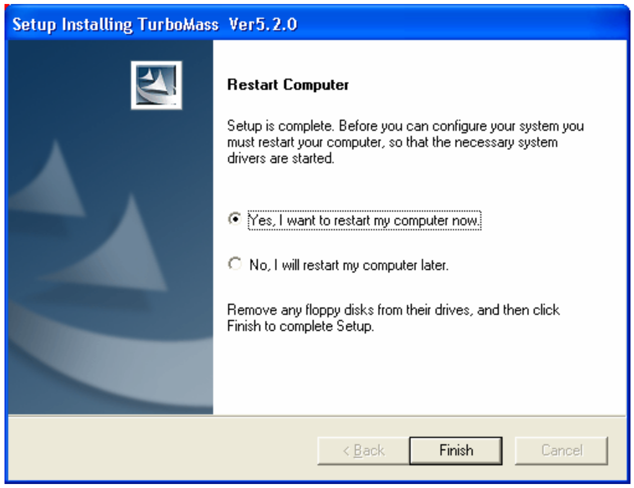
22. Click **Next** to continue with the installation.



When MATLAB completes, the following dialog appears:



23. Click **Close**, and the following appears:



24. The installation process finishes and prompts to reboot the computer. Leave the "**Yes, I want to restart my computer now.**" option checked and click **Finish**.

    When the system restarts, the TurboMass Software 5.2 startup icon will appear on the desktop.

    Turn on the mass spectrometer and wait 3 minutes for it to boot up. Double click on the TurboMass icon and then pump down the mass spectrometer.

Installing Clarus 500 MS NIST/EPA/NIH Library (2002)

If the NIST Library is currently installed, you do not need to reinstall. These instructions are provided for those who have not yet installed NIST.

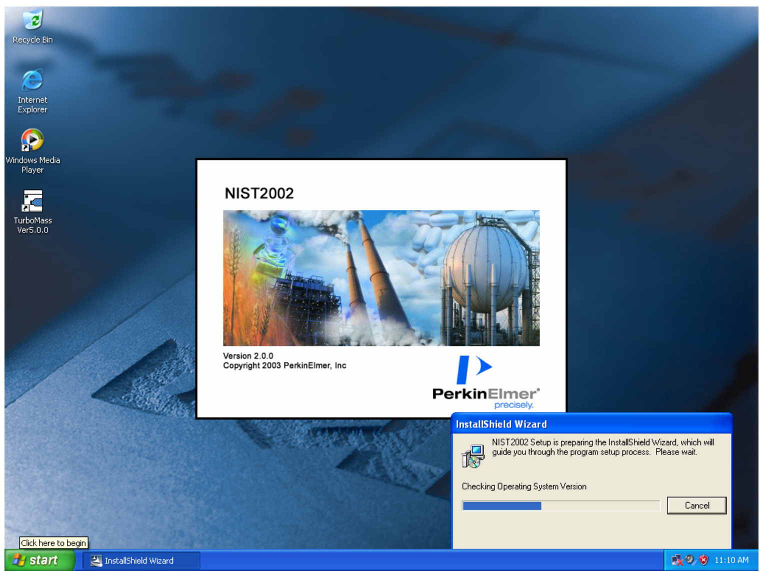
After installing the TurboMass software, you can install the NIST Library option next. The NIST Library software is sold and licensed separately from the TurboMass software.

NOTE: *Always refer to the Release Notes supplied with the NIST Library for the most up-to-date information.*

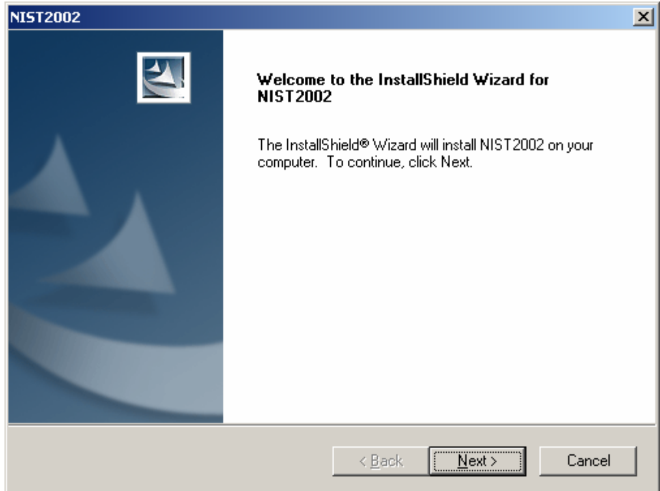
Installing the NIST Library

1. Insert the NIST install CD in the CD-ROM drive.

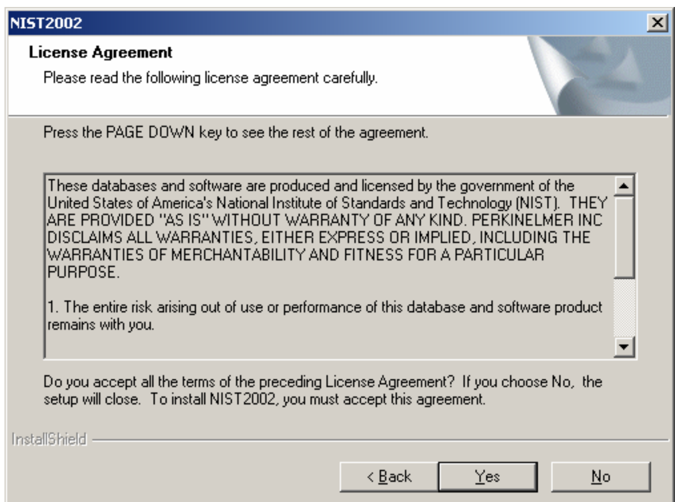
2. Right-click Start and Explore to use MS Explorer to display the contents of the CD drive. Click on Setup.exe to begin the install process.



The setup splash screen and setup screen are displayed:

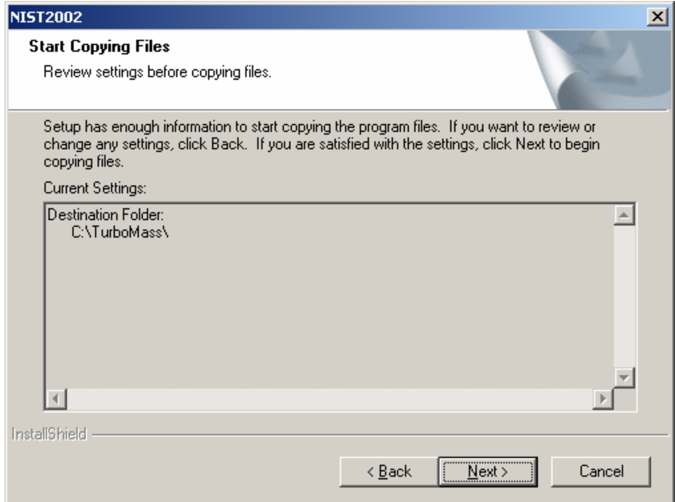


3. Click **Next>** to continue.

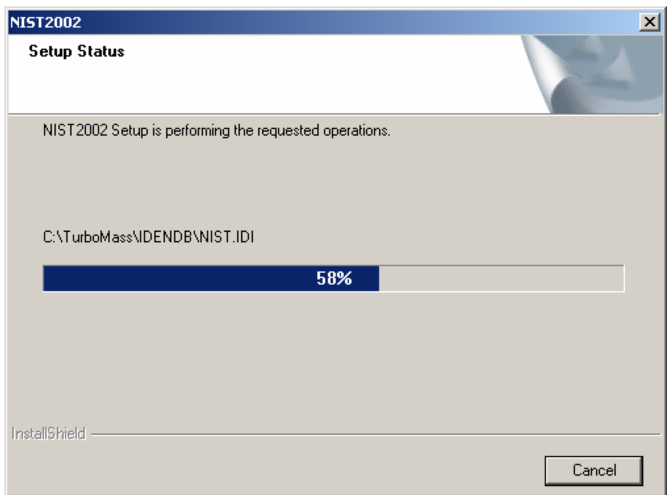


4. Click **Yes** to accept the terms of the licensing agreement and continue.

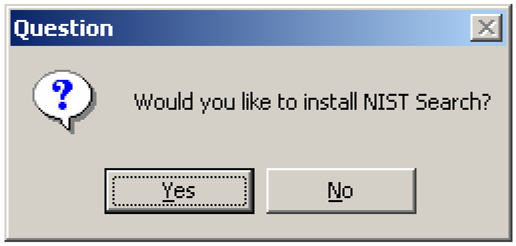
A screen indicating the install destination folder is displayed:



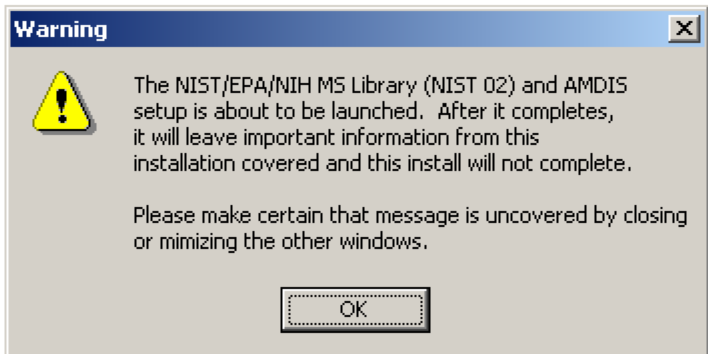
5. Click **Next>** to continue, and the software installation process begins.



A prompt next appears to install the NIST search; click **Yes**.



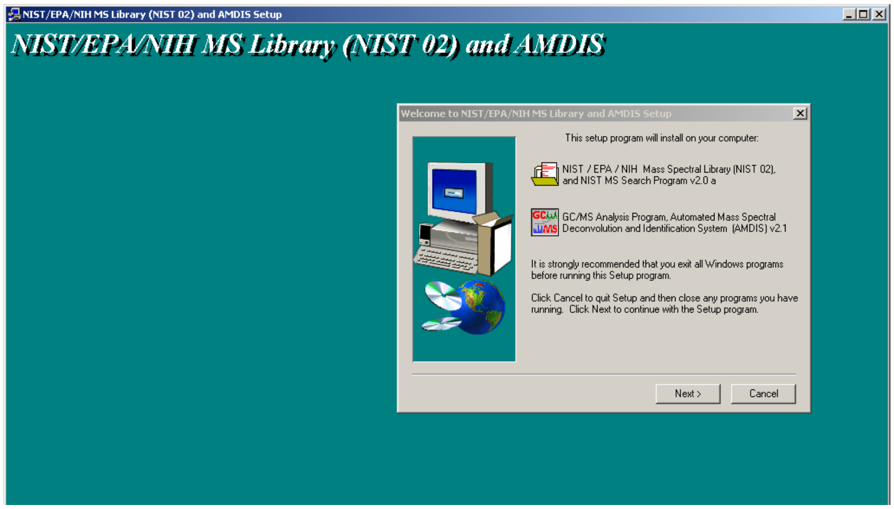
A warning is next displayed reminding the installer to close any open windows when the installation completes. These windows are left open by the install process and will cover the final prompt to close the NIST software installation.



NOTE: *Be sure to close open windows on the desktop and watch for this prompt at the end of the installation!*

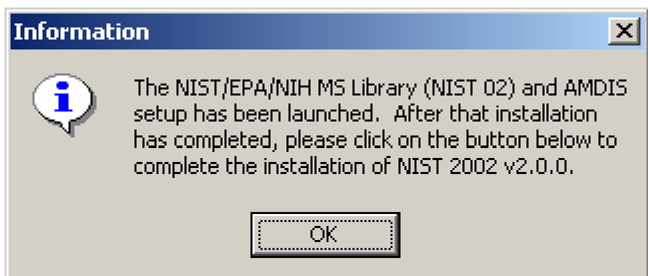
6. Click **OK**.

   The next screen prompts to continue the install process. Installation files are copied on the hard drive:

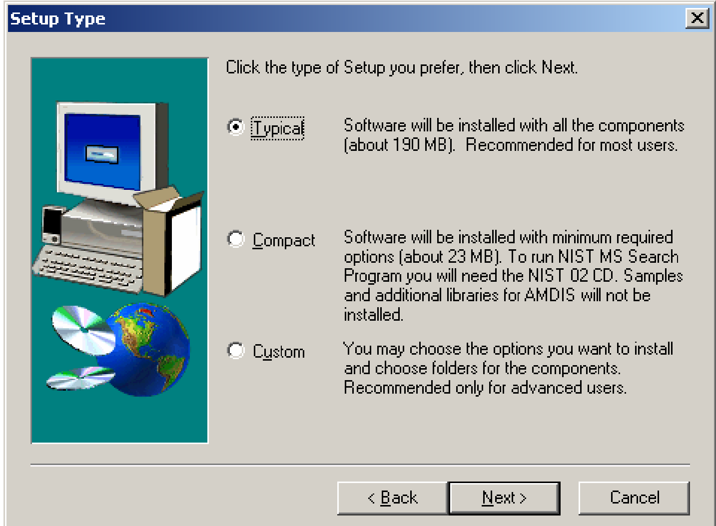


7. Click **Next>** to begin.

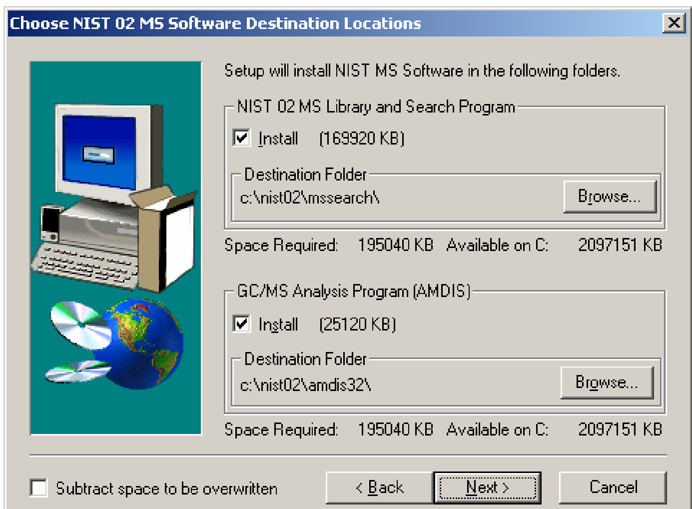
   The NIST install splash screen is displayed and the install process begins. The next screen prompts to finish the installation:



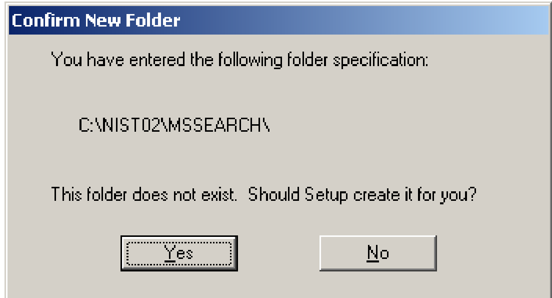
8. Click **OK**. When prompted for the setup type, leave the default **Typical** checked and click **Next>**:

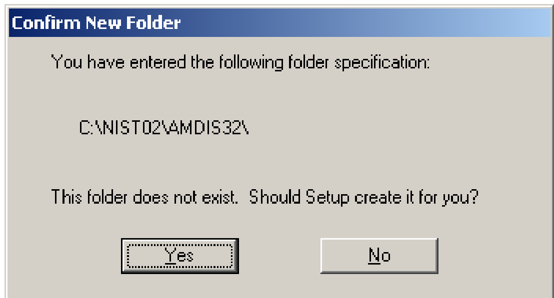


9. The next window displays the default install directories; leave the default options checked and click **Next>**:



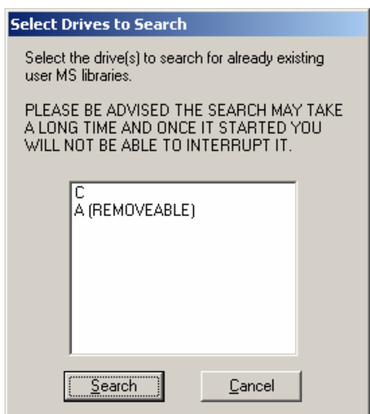
If the following folders do not exist, the system will prompt to create them:





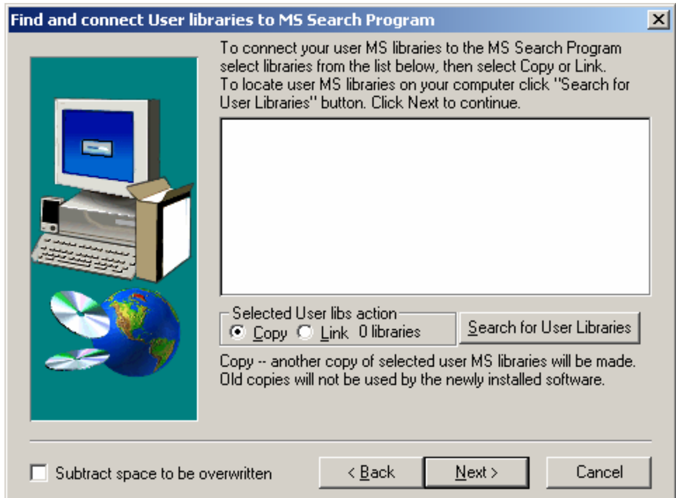
10. Click **Yes** to Confirm each new folder.

    The install process will next prompt to search the hard drive for any existing installed libraries:

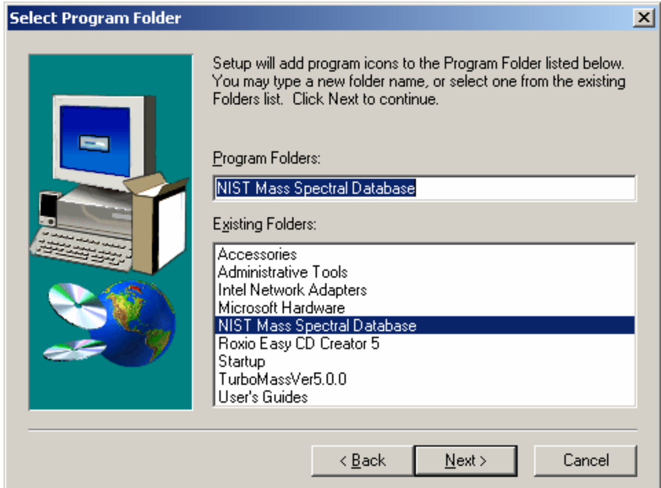


11. Click **Search**.

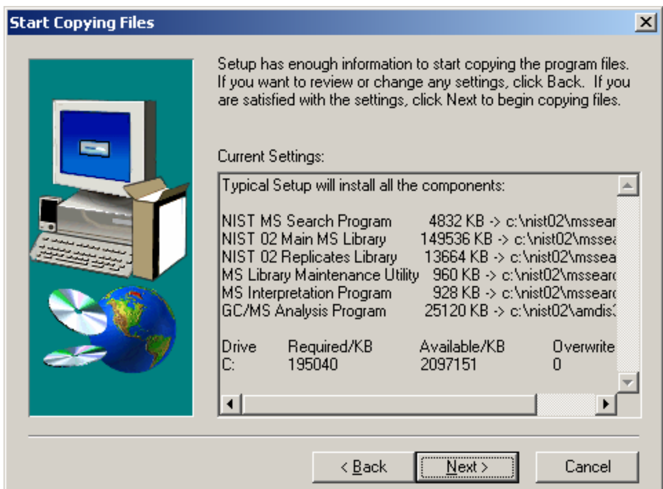
12. The next screen will prompt to connect any libraries found on the drive to the MS search program. If any libraries are displayed in the list, highlight the libraries that should be included in library searches, check **Copy or Link** and click **Next>** to continue.



13. A prompt appears for the program folder location. Accept the default entry and click **Next>**.

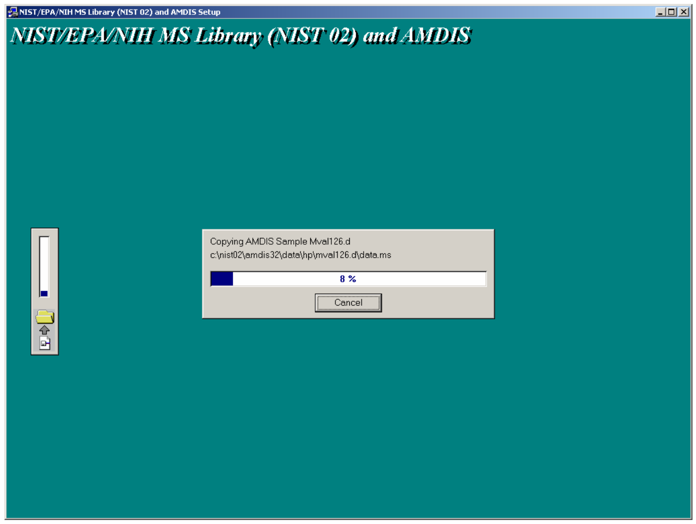


A final review of the install options is displayed:

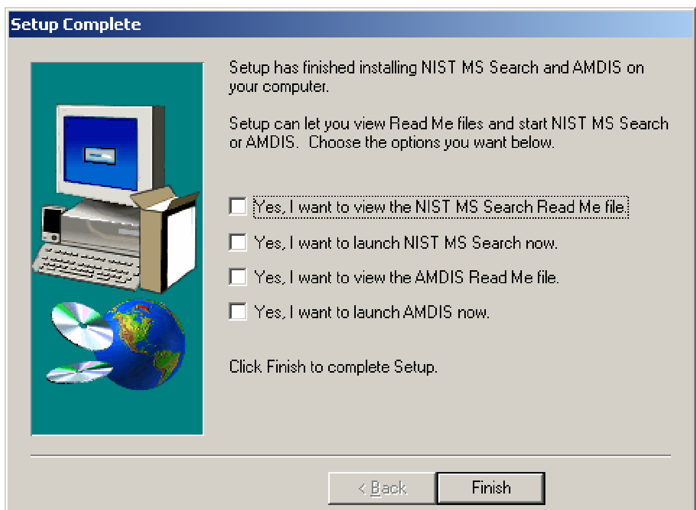


14. Click **Next>** to continue.

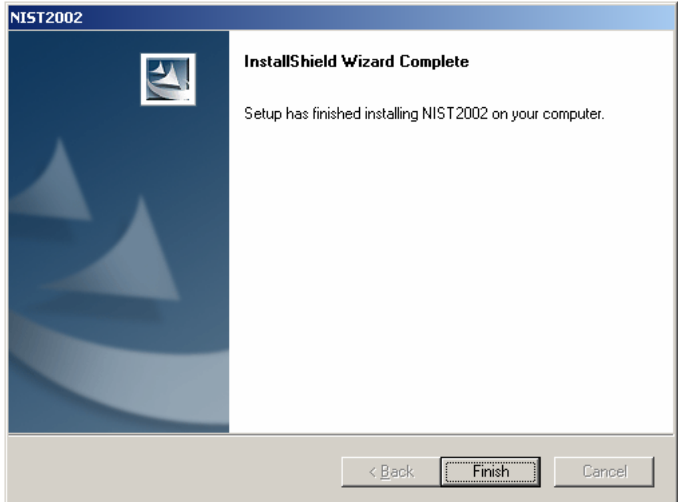
    The installation of the MS Search program begins and runs to completion:



15. When the MS Search software install is complete, a screen is displayed prompting you to view Read-Me files. If you wish to view one or more files at this point, check the appropriate box(es) and click **Finish**.



The installation process completes and closes. Be sure to close all open windows and find the final prompt screen indicating the install process is complete:



16. Click **Finish** to close the NIST installation process.

Configuring TurboMass for GC Control

Before you begin to use TurboMass for the first time, you must first configure it (or verify that it is configured) to interact with the Clarus 500 GC.

After establishing communication between the instruments in the system and creating your GC method, you can develop your TurboMass method.

The procedure used to configure the GC depends upon whether you are initially configuring TurboMass for GC control or are making front panel changes to the GC.

- **Initial GC Configuration:** To set up the LINK and GC for TurboMass control for the first time.

- **Reconfiguring the GC:** To make front panel or hardware changes to the GC without changing the LINK configuration. Reconfiguration is also required if you add an autosampler.

Configuring the GC for the First Time

The following steps summarize the procedure for configuring TurboMass for GC control the first time:

1. Display the top level (main) window.

2. Select an interface.

3. Select **Configure** from the *GC* menu.

4. Verify the Data Acquisition port.

5. Set the *LINK Configuration* Options.

6. Set the *GC Configuration* Options.

To configure the Clarus 500 GC:

In the top-level window, **Select Inlet Interface** from the Configure menu.

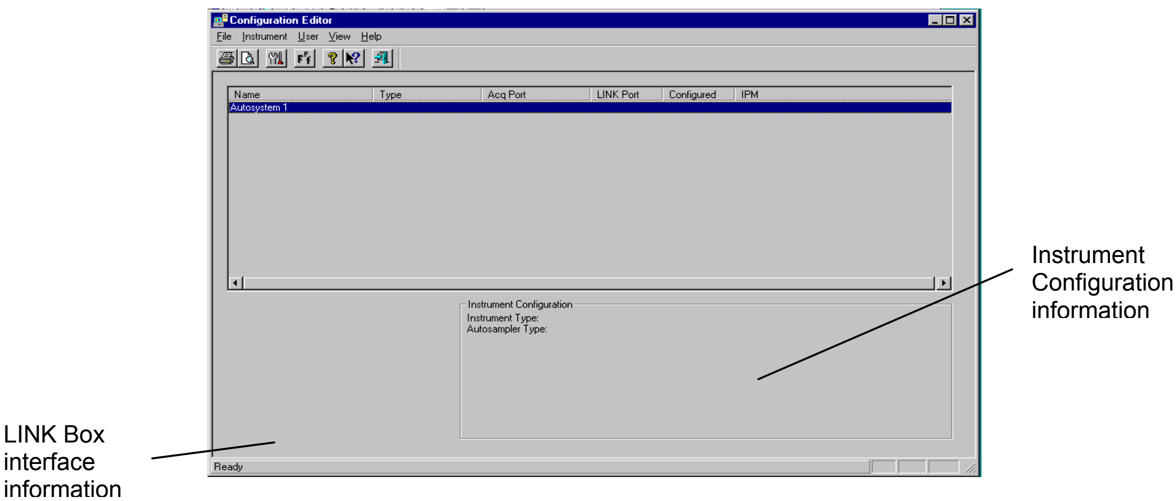
1. If the **Clarus 500** is not selected (highlighted), click to select it.

2. Click **OK**.

   All GC commands are accessible from the **GC** menu in the top-level window. From this menu you can set up your GC configuration, develop your GC method, work interactively with the GC, and execute all other GC related procedures.

3. From the *GC* menu, select **Configure**.

   The *Configuration Editor* summary window is displayed. This displays the GC information that will be defined during configuration.



After configuring the GC, the area below the Configuration Editor summary list displays key GC information. The box on the left contains information about the LINK interface, which includes the type (model number), EPROM version number, memory size available in the interface (in bytes), and serial number. The box on the right contains a summary of the GC configuration.

Summary of information displayed on the Configuration Editor window:

Field	Description
Name	The name of the GC.
Type	The GC model or type.
Acq Port	The physical data acquisition port to which the 600 Series LINK Interface is connected.
LINK Port	The physical port in the LINK interface to which the GC is connected.
Configured	Displays **YES** if you provided all the information needed to configure the GC. Otherwise, **NO** is displayed.
IPM	Displays **YES** if the Instrument Personality Module (IPM) for the GC has been downloaded. The first time you open this window, the IPM will not have been downloaded.

4. From the *Configuration Editor* window, select **Configure** from the *Instrument* menu.

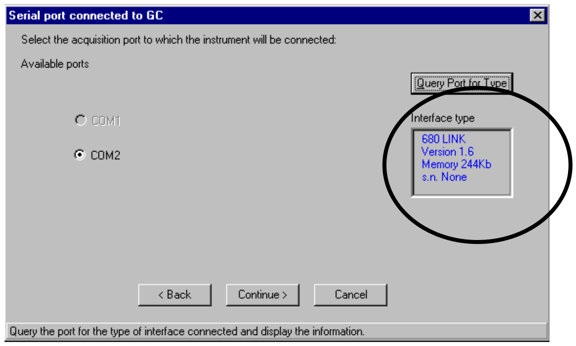
   The serial port connected to GC dialog is displayed.

5. Verify the serial port (in this example, COM2), LINK box connection, and firmware version.

NOTE: *If the mass spectrometer and your computer were configured for COM1, then COM1 is your serial port.*

6. Click on the **Query Port** for *Type* button.

   The Interface type is displayed in the box.



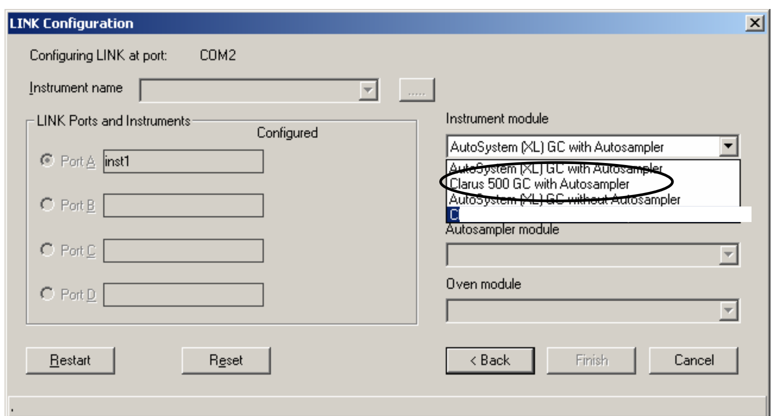
7. Click the **Continue** button.

   The *LINK Configuration* dialog with the COM port and instrument name displays.

8. Select **Port A** from the **LINK Ports and Instruments** list:
   inst1 is displayed in the box to the right of Port A.

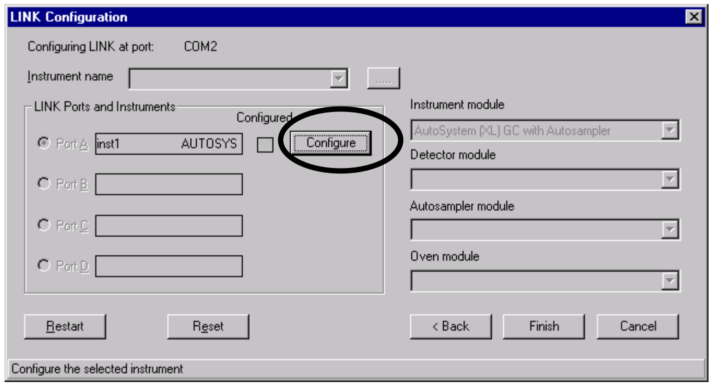
9. Select the **Clarus 500 GC with Autosampler** in the *Instrument Module* list.

   If your Clarus 500 GC has an autosampler, select **Clarus 500 GC with Autosampler** even if you won't be using the autosampler. You can change this setting from the *Method Editor*.



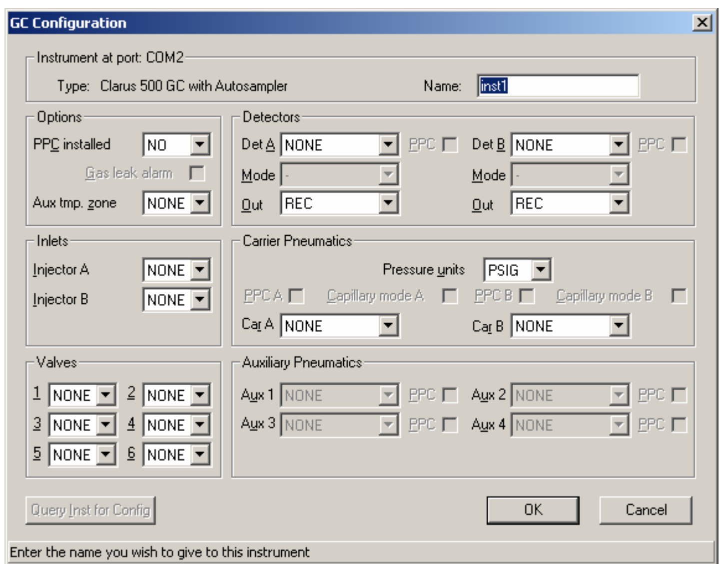
If you make a mistake, click **Restart**. This disconnects the GC and clears the LINK port. Clicking **Reset** clears all the changes to this dialog and returns it to the state it was in before you opened it.

When the software verifies this connection, a box appears under **Configured** and a **Configure** button appears.



10. In the *LINK Configuration* dialog, click the **Configure** button next to the port selection.

    The *GC Configuration* dialog is displayed.

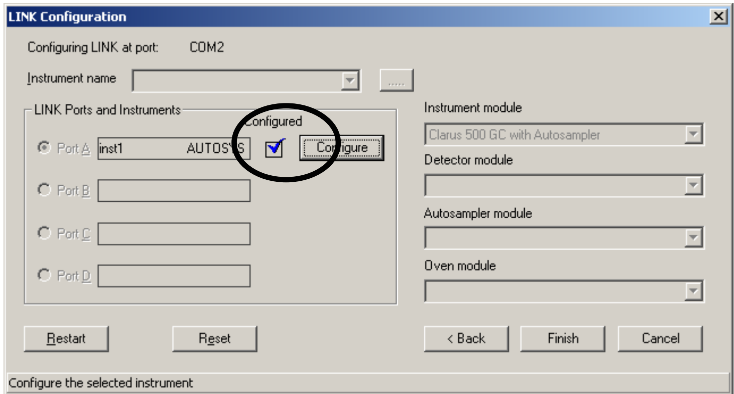


11. To rename the GC to something other than its default name (*inst1*), enter the new name in the *Name* text box.

    This name will appear under the *Name* field in the *Configuration Editor* window.

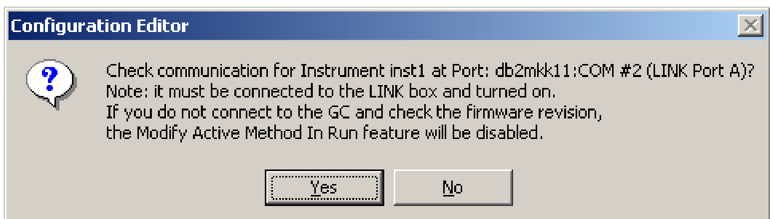
12. Click **OK**.

    A check mark in the *LINK Configuration* dialog indicates that the GC has been configured.



13. Click **Finish**.

    When you first configure the GC, the following message may display:

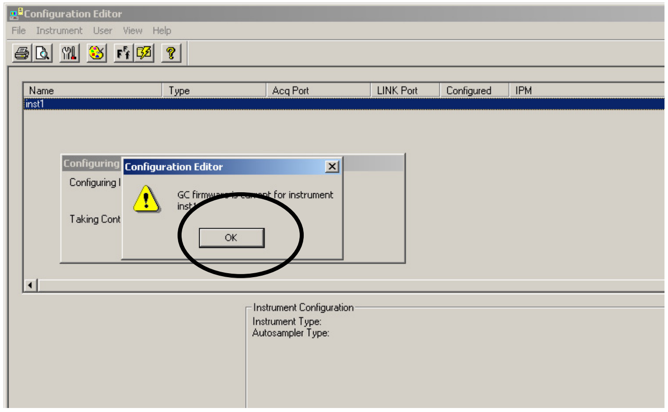


14. If the GC is not turned on, turn it on now and then click **Yes**.

    OR

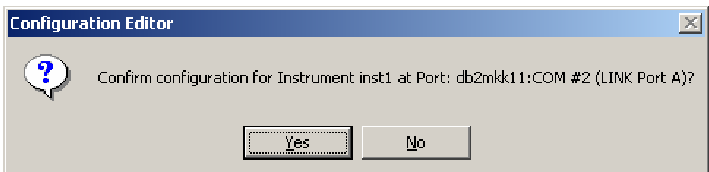
    If the GC is connected and turned on, click **Yes**.

The following message is displayed:



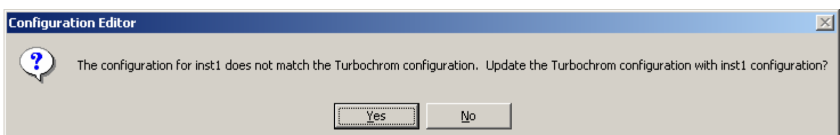
15. Click **OK**.

    The following message is displayed:



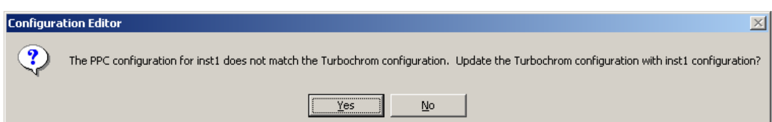
16. Click **Yes**.

    The following message is displayed:



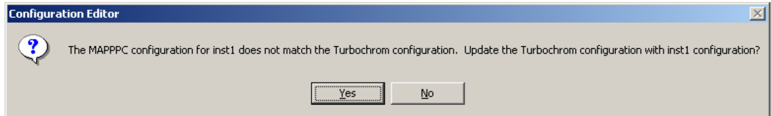
17. Click **Yes**.

    If your Clarus 500 GC has PPC, the following message is displayed:



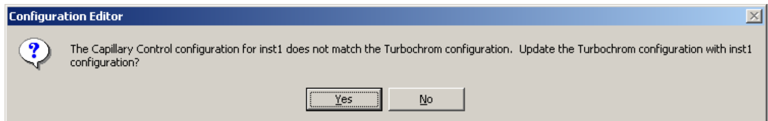
18. Click **Yes**.

    The following message is displayed:



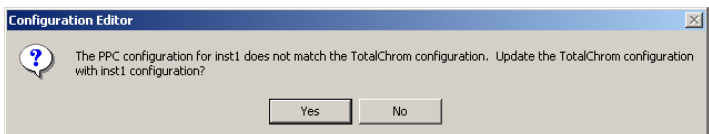
19. Click **Yes**.

    The following message is displayed:



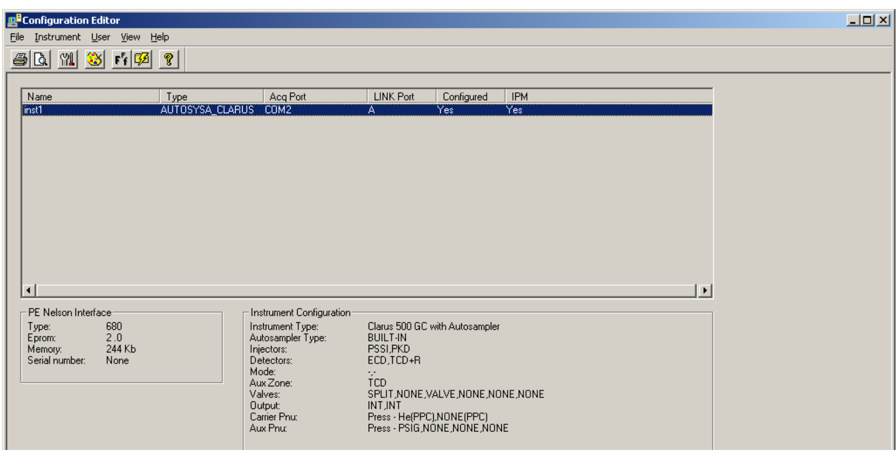
20. Click **Yes**.

    The following message is displayed:



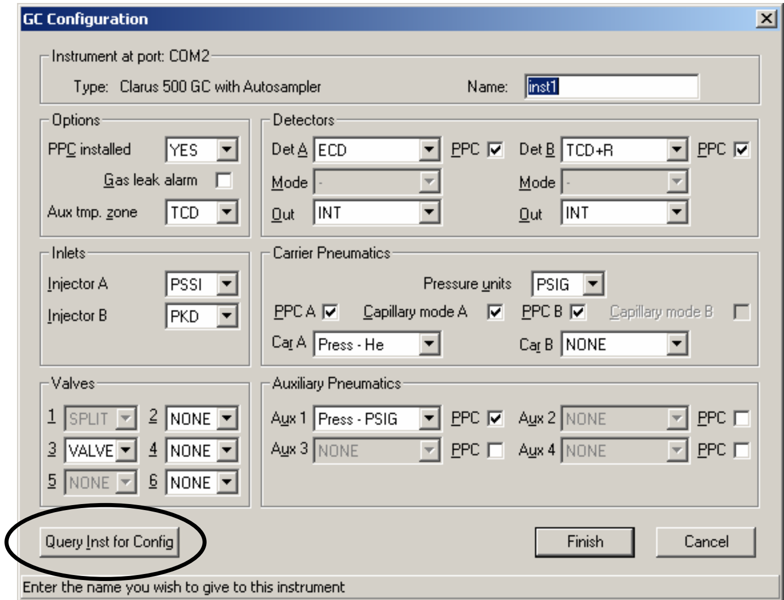
21. Click **Yes**.

    The following screen is displayed:



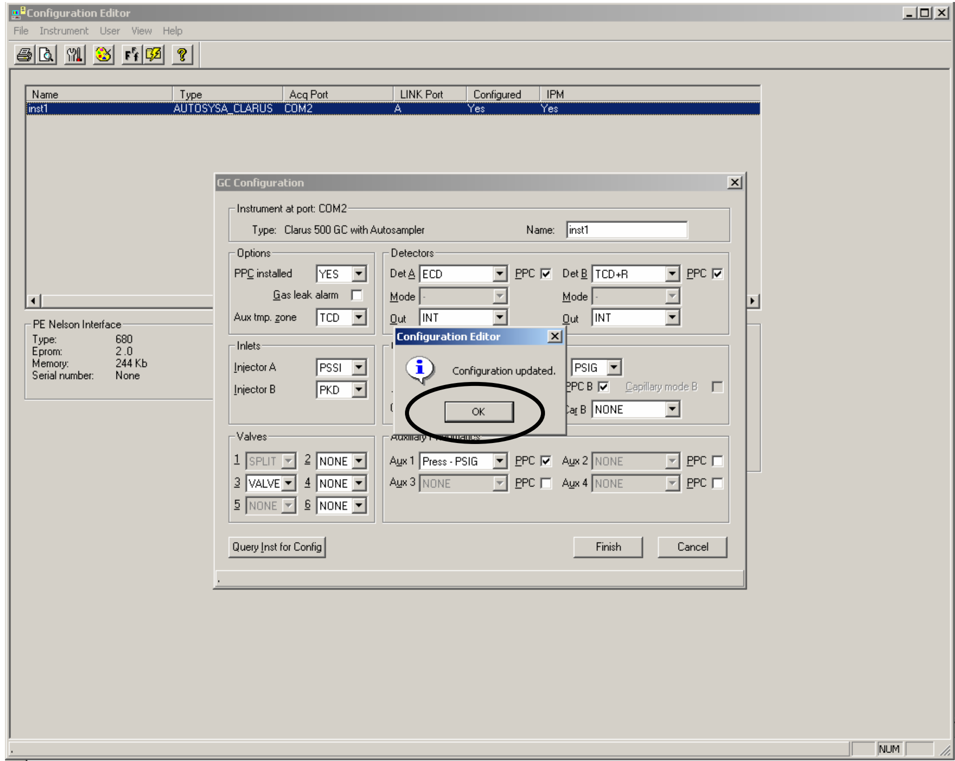
22. Select **Configure** from the *Instrument* menu.

    The following screen is displayed.



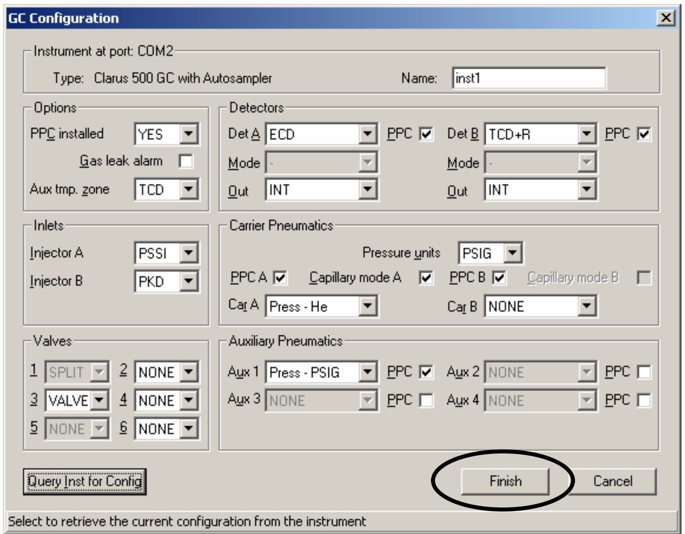
23. Click the **Query Inst for Config** button.

The following screen is displayed.

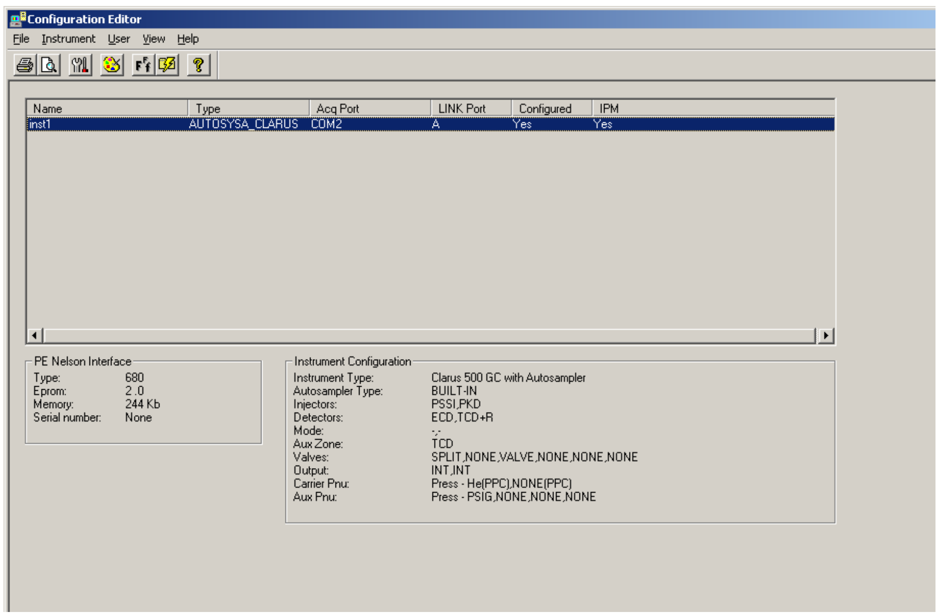


24. Click **OK**.

    The *Configuration Editor* window is updated and your instrument is now configured and the GC Configuration screen displays.



25. Click **Finish.**



26. Close the *Configuration Editor* by selecting **Exit** from the File menu.

Appendix C TurboMass Quantify Calculations

TurboMass Quantify Calculations

Peak Response

There are two main methods of calculating peak response value, these are External Standard and Internal Standard. The calibration base can be either Area or Height, the examples below are shown for Area.

External

$$\text{Peak Response} = \text{Area}$$

Where:
Area is the area of a peak calculated by peak detection.

Internal

$$\text{Peak Response} = \frac{\text{Area} * \text{Amount}_I}{\text{Area}_I}$$

Where:
Area is the area of a peak calculated by peak detection.
Amount_I is the given amount of the Internal Standard in the sample
Area_I is the area of the internal standard peak calculated by peak detection.

Calibration Curve Calculations

TurboMass can fit several types of calibration curves which are described below.

Weighted Calibration Curves

Calibration points used when fitting curves can be given a weighted importance, the larger the weighting the more significant a point is treated when the curve is fitted.

Weighting (w_i) of i^{th} calibration point is calculated using one of the following, all w_i are set to 1 for no weighting.

1) $w_i = y_i^{-1}$
2) $w_i = y_i^{-2}$
3) $w_i = x_i^{-1}$
4) $w_i = x_i^{-2}$

Where:
y_i is Y value (response) of i^{th} calibration point
x_i is X value (concentration) of i^{th} calibration point

Include Origin

If Include Origin is selected as a calibration curve type an extra point with zero concentration and response is used in the regression. The extra point has a weighting of 1.

Average RF

The calibration curve formed is linear passing through the origin with a gradient equal to the average response values of the calibration points.

$$\text{Average RF} = \frac{Swy}{Sw}$$

Where:

$$Swy = \Sigma \frac{y_i * w_i}{x_i}$$

$$Sw = \Sigma\ w_i$$

y_i is Y value (response) of i^{th} calibration point

x_i is X value (concentration) of i^{th} calibration point

w_i is weighting of i^{th} calibration point, all set to 1 for no weighting.

Linear

The calibration curve is formed by fitting a line using linear regression to a set of calibration points.

$$\text{Gradient} = Swxy / Swxx$$
$$\text{Intercept} = y_{w,mean} - \text{Gradient} * x_{w,mean}$$

Where:

$$y_{w,mean} = \frac{\Sigma\ y_i * w_i}{\Sigma w_i}$$

$$x_{w,mean} = \frac{\Sigma\ x_i * w_i}{\Sigma w_i}$$

Swxy = $\Sigma (x_i - x_{w,mean}) * (y_i - y_{w,mean})$

Swxx = $\Sigma (x_i - x_{w,mean})^2$

y_i is Y value (response) of i^{th} calibration point

x_i is X value (concentration) of i^{th} calibration point

w_i is weighting of i^{th} calibration point, all set to 1 for no weighting.

If Force Origin is selected a line with zero intercept is fitted.

$$\text{Gradient} = \frac{\Sigma x_i * y_i * w_i}{\Sigma x_i^2 * w_i}$$

Quadratic and Higher Order Curves

TurboMass uses a general Least Squares Fit algorithm to regress a polynomial of any order against the calibration points. The method used is outlined below.

Polynomial regression can be described as the fitting of m "independent" variables (Xj, j = 0 to m-1) to a single "dependent" variable y. i.e.

$$\mathbf{y} = \mathbf{Xb} + \mathbf{e}$$

where **y** is the *n* x 1 vector containing the n y values (y_i), **X** is the *n* x *m* matrix of x values, (x_i^j), **b** is the *m* x 1 vector of regression coefficients (b_i), and **e** is the *n* x 1 vector of residuals from the fit to each y_i value.

The familiar least squares solution for the regression coefficients is given by:

$$\mathbf{b} = (\mathbf{X'X})^{-1}\mathbf{X'y}$$

where $^{-1}$ indicates matrix inverse, and ' indicates matrix transpose.

The above equation can then be solved using Gauss-Jordan elimination.

To implement weighted regression **X** and **y** are first multiplied by a diagonal *n* x *n* matrix **P** (i.e. **X** becomes **PX** and **Y** becomes **PY**), before the above equation is solved.

where each element (pij) of **P** is given by:

$$p_{ij} = w_i^{1/2} \quad \text{for } i = j$$

$$p_{ij} = 0 \quad \text{for } i <> k$$

w_i is weighting of i^{th} calibration point, all set to 1 for no weighting.

Peak Amount Calculations

User Specified Response Factor

If a user response factor if selected within the quantitation method calibration curves are not used. The following calculation is performed to obtain peak amounts.

$$\text{Amount} = \frac{\text{Peak Response}}{\text{Response Factor}}$$

Where:
Peak Response is the response value calculated for a peak.
Response Factor is user entered response factor for that compound.

Average RF Calibration Curve

Amounts are calculated using an Average RF calibration as follows

$$\text{Amount} = \frac{\text{Peak Response}}{\text{Average RF}}$$

Where:
Peak Response is the response value calculated for a peak.
Average RF is average response factor calculated for a set of calibration points.

Linear Calibration Curve

Amounts are calculated using a linear calibration as follows

$$\text{Amount} = \frac{\text{Peak Response - Intercept}}{\text{Gradient}}$$

Where:
Peak Response is the response value calculated for a peak.
Intercept is the intercept calculated for the linear calibration.
Gradient is the gradient calculated for the linear calibration.

Quadratic and Higher Order Calibration Curves

Amounts are calculated by solving the following equation using the Newton-Raphson Method.

$$\text{Peak Response} = \text{P (Amount)}$$

Where:
Peak Response is the response value calculated for a peak.
P( ) is the polynomial function calculated for a set of calibration points.

User Parameters

User parameters can be used to multiply or divide the final quantitation results. These factors are entered per sample in the Sample List. If a factor is not specified of zero it is assumed to be one.

$$\text{Final Amount} = \frac{\text{Amount * Dilution Factor * Extract Volume * User Factor}}{\text{Initial Amount * Injection volume}}$$

The User Peak Factor is entered per compound in the Quantify Method.

$$\text{Final Amount} = \text{Amount * User Peak Factor}$$

Calibration Curve Statistics

Coefficient of Determination

The coefficient and determination is calculated for a regressed calibration curve. In the case of a linear unweighted curve it is equivalent to the square of the correlation coefficient and is reported as such. Correlation coefficients are not a valid statistic for any other type of regressed curve.

For each data point a value of y ($y_{i,pred}$) can be predicted from the calibration curve at the position x_i. For each data point a residual between the actual and predicted y value can be calculated as ($y_i - y_{i,pred}$), and the residual sum of squares (RSS) can be calculated as:

$$RSS = \Sigma (y_i - y_{i,pred})^2$$

The total variation in the data is reflected in the corrected sum of squares (CSS), calculated as:

$$CSS = \Sigma (y_i - y_{mean})^2$$

where y_{mean} is the mean value of y.

The model sum of squares (MSS) is the portion of the total variation accounted for by the regression, i.e.

$$MSS = CSS - RSS$$

The coefficient of determination (r^2) is the proportion of the variation accounted for by regression, and is given by the ration of the model sum of squares to the corrected sum of squares, i.e.

$$\begin{aligned} r^2 &= MSS / CSS \\ &= (CSS - RSS) / CSS \end{aligned}$$

Curve Correlation Coefficient

The correlation coefficient is only a valid statistic of fit for regressed unweighted linear curves. In this case the square of the correlation coefficient is equivalent to the coefficient of determination described above.

Internal

$$\text{Peak Response} = \frac{\text{Area} * \text{Amount}_I}{\text{Area}_I}$$

Where:
Area is the area of a peak calculated by peak detection.
Amount_I is the given amount of the Internal Standard in the sample
Area_I is the area of the internal standard peak calculated by peak detection.

Appendix D
Sample and Compound Table Output Fields

Compound and Sample Report Output Fields

The following table describes each output field and format. The two columns on the right specify whether the field is available in the Compound Report (C) and/or Sample Report (S).

Field Name	**Field ID**	**Format**	**Description**	**Format**	**C**	**S**
Acquired Date	RAW_DATE	C 9	Date raw data acquired	DD-MMM-YY	•	
Acquired Time	RAW_TIME	C 8	Time raw data acquired	HH:MM:SS	•	
Blank Sub. Conc.			Concentration found in Blank which is subtracted from final Concentration		•	•
Calibration Date	CDB_DATE	C 9	Date Quantify Calibration last modified	DD-MMM-YY	•	•
Calibration File	CDB_NAME	C 8	Name of Quantify Calibration file used to quantify peak; excludes extension		•	•
Calibration Time	CDB_TIME	C 8	Time Quantify Calibration last modified	HH:MM:SS	•	•
Trace	QUAN_TRACE	C 40	Raw datafile chromatogram integrated to produce peak. A chromatogram description can consist of 'TIC', 'BPI', mass or mass range. To add or subtract chromatograms use '+' and '-' operators		•	•
Concentration Deviation			% error from standard concentration 100*(Conc-StdConc)/StdConc		•	•
Pk Flags	PK_FLAGS	C 4	Peak integration description flags: 1st character= baseline start, 2nd = baseline end **b** = starts/ends on chromatogram curve **v** = starts/ends as valley dropline between two peaks **s** = starts/ends as a shoulder dropline between two peaks **t** = perk was not detected within the retention time window **M** = manually defined by user		•	
Found Peak Scan			Scan number of the peak apex		•	

Field Name	Field ID	Format	Description	Format	C	S
Injection Volume	INJ_VOL	N 19.9	Injection volume of sample, currently set-up to 1. Set during Quantify Locate processing, otherwise is 0		•	
IS Area			Area of internal standard compound		•	•
IS Compound #			Compound reference number of internal standard		•	•
IS Found RT			Found retention time of internal standard compound		•	•
IS Height			Height of internal standard compound		•	•
Modified Date	MOD_DATE	C 9	Date peak baseline last manually modified	DD-MMM-YY	•	•
Modified Time	MOD_TIME	C 8	Time peak baseline last manually modified	HH:MM:SS	•	•
Modify Comment	MOD_TEXT	C 40	Modification description entered for last peak baseline modification		•	•
Modify User	MOD_USER	C 16	Name of user who last manually modified peak baseline. This is the user login name		•	•
Peak Height			Height of the target compound		•	•
Peak Mass			Unused		•	•
Predicted RRT			Calculated relative retention time			•
Predicted RT			Compound retention time from Quantify Method			•
Sample CONDITIONS		Char (255)	Condition information from Sample List. Recorded in data file header		•	
Sample TASK		Char (50)	Task description from Sample List. Recorded in data file header		•	
Sample Text (FILE_TEXT)		Char (255)	Sample text description from Sample List. Recorded in data file header		•	

Field Name	Field ID	Format	Description	Format	C	S
USER_DIVISOR_1		Double	Divisor used during concentration calculation stage of Quantify. Defaults to 1 if not specified		●	
USER_FACTOR_1 … USER_FACTOR_3		Double	Multipliers used during concentration calculation stage of Quantify. Defaults to 1 if not specified		●	
User Peak Factor			User Peak Factor set in the Quantify method		●	●
User Peak RF			User RF Value set in the Quantify method		●	●

Field Name	Format	Description	Version Added
PKAREAPER	N 10.2	Quantify Mass chromatogram Integrated Peak Area	5.0
NPKAREPER	N 10.2	Normalized Quantify Mass chromatogram Integrated Peak Area	5.0
QNTRATIO	N 19.9	Quantify Mass chromatogram Ratio to Largest Peak area	5.0
QNTLOWLIM	N 19.9	Quantify Mass chromatogram Ratio Low Limit	5.0
QNTHIGLIM	N 19.9	Quantify Mass chromatogram Ratio High Limit	5.0
QNTPERTOL	N 19.9	Quantify Mass chromatogram Ratio % Tolerance	5.0
QNTMLTPAS	L	TRUE if within the limits	5.0
ION1MASS	N 10.2	Qualifier Ion #1 Mass	5.0
ION1RT	N 8.3	Qualifier Ion #1 Mass Chromatogram Peak Top Retention Time	5.0
ION1AREA	N 16.3	Qualifier Ion #1 Mass chromatogram Integrated Peak Area	5.0
ION1HEIGHT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height	5.0
ION1_ST_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline Start	5.0
ION1_EN_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline End	5.0
ION1_ST_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline Start	5.0
ION1_EN_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline End	5.0
ION1RATIO	N 19.9	Qualifier Ion #1 Ratio	5.0
ION1LOWLIM	N 19.9	Qualifier Ion #1 Ratio Low Limit	5.0
ION1HIGLIM	N 19.9	Qualifier Ion #1 Ratio High Limit	5.0

Field Name	Format	Description	Version Added
ION1PERTOL	N 19.9	Qualifier Ion #1 Percent Tolerance	5.0
ION1PASS	L	TRUE if within the limits	5.0
ION2MASS	N 10.2	Qualifier Ion #1 Mass	5.0
ION2RT	N 8.3	Qualifier Ion #1 Mass Chromatogram Peak Top Retention Time	5.0
ION2AREA	N 16.3	Qualifier Ion #1 Mass chromatogram Integrated Peak Area	5.0
ION2HEIGHT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height	5.0
ION2_ST_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline Start	5.0
ION2_EN_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline End	5.0
ION2_ST_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline Start	5.0
ION2_EN_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline End	5.0
ION2RATIO	N 19.9	Qualifier Ion #1 Ratio	5.0
ION2LOWLIM	N 19.9	Qualifier Ion #1 Ratio Low Limit	5.0
ION2HIGLIM	N 19.9	Qualifier Ion #1 Ratio High Limit	5.0
ION2PERTOL	N 19.9	Qualifier Ion #1 Percent Tolerance	5.0
ION2PASS	L	TRUE if within the limits	5.0
ION3MASS	N 10.2	Qualifier Ion #1 Mass	5.0
ION3RT	N 8.3	Qualifier Ion #1 Mass Chromatogram Peak Top Retention Time	5.0
ION3AREA	N 16.3	Qualifier Ion #1 Mass chromatogram Integrated Peak Area	5.0
ION3HEIGHT	N 12.2	Qualifier Ion #1 Mass chromatogram Integrated Peak Height	5.0
ION3_ST_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline Start	5.0
ION3_EN_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline End	5.0
ION3_ST_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline Start	5.0
ION3_EN_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline End	5.0
ION3RATIO	N 19.9	Qualifier Ion #1 Ratio	5.0
ION3LOWLIM	N 19.9	Qualifier Ion #1 Ratio Low Limit	5.0
ION3HIGLIM	N 19.9	Qualifier Ion #1 Ratio High Limit	5.0
ION3PERTOL	N 19.9	Qualifier Ion #1 Percent Tolerance	5.0
ION3PASS	L	TRUE if within the limits	5.0

Field Name	Format	Description	Version Added
ION4MASS	N 10.2	Qualifier Ion #1 Mass	5.0
ION4RT	N 8.3	Qualifier Ion #1 Mass Chromatogram Peak Top Retention Time	5.0
ION4AREA	N 16.3	Qualifier Ion #1 Mass chromatogram Integrated Peak Area	5.0
ION4HEIGHT	N 12.2	Qualifier Ion #1 Mass chromatogram Integrated Peak Height	5.0
ION4_ST_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline Start	5.0
ION4_EN_RT	N 8.3	Qualifier Ion #1 Mass chromatogram Integrated Peak RT of Baseline End	5.0
ION4_ST_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline Start	5.0
ION4_EN_HT	N 12	Qualifier Ion #1 Mass chromatogram Integrated Peak Height of Baseline End	5.0
ION4RATIO	N 19.9	Qualifier Ion #1 Ratio	5.0
ION4LOWLIM	N 19.9	Qualifier Ion #1 Ratio Low Limit	5.0
ION4HIGLIM	N 19.9	Qualifier Ion #1 Ratio High Limit	5.0
ION4PERTOL	N 19.9	Qualifier Ion #1 Percent Tolerance	5.0
ION4PASS	L	TRUE if within the limits	5.0
CLSTMULTRT	L	TRUE if this is the closest Peak to the Retention time (that does not pass the ratio tests	5.0
DATASOURCE	N 2	0 = MS, 1 = GC CHAN1, 2 = GC CHAN2	5.1
INVALIDCNC	L	TRUE if there was something wrong with the internal standard data	5.1
EPA_CONC	N 29.9	Adjusted Concentration	5.2
SPIKERECOV	N 19.9	Matrix Spike / Matrix Spike Duplicate Recovery	5.2
RPD	N 19.9	Relative Percent Difference	5.2
MATRIXTYPE	N 1	0 = Soil, 1 = Water	5.2
EPAQUALTXT	C 11	EPA Qualifier Ions	5.2
EPA_MCONC	N 29.9	Moisture Adjusted Concentration	5.2

Field Name	Format	Description	Version Added
GOODEPACAL	N 10	Bit Fields 1 if valid/operation performed, 0 if not Valid Adjusted Concentration 0x00000001 Valid Moisture Adjusted Concentration 0x00000002 Valid Matrix Spike Recovery 0x00000004 Valid Matrix Spike RPD 0x00000008 EPA FLAG Manually Changed 0x00000010	5.2

Appendix E
LIMS Import File
Example

Example of a Sample List Import File

[System Description]
Description=EXAMPLE SIF FILE
MaxNoOfSamples=250

[Constant Parameters]
BatchID=InitialCalibration (Sample List Filename)

(From the list below build a cross reference map relating the intems in the Data section to Sample list entries. Build a new INTERNAL Sample record and append it to the newly created sample list file.)

[Variable Parameter List]
NumberOfParameters=56
Parameter1=FILE_NAME
Parameter2=FILE_TEXT
Parameter3=MS_FILE
Parameter4=MS_TUNE_FILE
Parameter5=INLET_FILE
Parameter6=INLET_PRERUN
Parameter7=INLET_POSTRUN
Parameter8=INLET_SWITCH
Parameter9=AUTO_FILE
Parameter10=PROCESS
Parameter11=PROCESS_PARAMS
Parameter12=PROCESS_OPTIONS
Parameter13=SAMPLE_LOCATION
Parameter14=JOB
Parameter15=TASK
Parameter16=USER
Parameter17=SUBMITTER
Parameter18=CONDITIONS
Parameter19=TYPE
Parameter20=ID
Parameter21=CONC_A
Parameter22=CONC_B
Parameter23=CONC_C
Parameter24=CONC_D
Parameter25=CONC_E
Parameter26=CONC_F
Parameter27=CONC_G
Parameter28=CONC_H
Parameter29=CONC_I
Parameter30=CONC_J

Parameter31=CONC_K
Parameter32=CONC_L
Parameter33=CONC_M
Parameter34=CONC_N
Parameter35=CONC_O
Parameter36=CONC_P
Parameter37=CONC_Q
Parameter38=CONC_R
Parameter39=CONC_S
Parameter40=CONC_T
Parameter41=FRACTION_MASS
Parameter42=INJ_VOL
Parameter43=STOCK_DIL
Parameter44=USER_DIVISOR_1
Parameter45=USER_FACTOR_1
Parameter46=USER_FACTOR_2
Parameter47=USER_FACTOR_3
Parameter48=SPARE_1
Parameter49=SPARE_2
Parameter50=SPARE_3
Parameter51=SPARE_4
Parameter52=SPARE_5
Parameter53=QUANT_METHOD
Parameter54=QUANT_CALFILE
Parameter55=QUAL_METHOD
Parameter56=REPORT_METHOD

[Variable Parameter Data]
NumberOfDataValues=2

Data1=Filena'me,file"text,MSFile,MsTuneFile,InletFile,InletPreRun,INletPostRun,InletSwitch,AutoFile,Process,ProcessParam,ProcessOptions,SampleLocation,Job,Task,User,Submitter,Conditions,Standard,ID,-12,1.2,1.3,1.4,1.5,1.6,1.7,1.8,1.9,2.0,2.1,2.2,2.3,2.4,2.5,2.6,2.7,2.8,2.9,3.0,12345.67890,1.25,1.0,1.0,1.0,2.0,3.0,Spare1,Spare2,Spare3,Spare4,Spare5,QuantMethod,QuantCalfile,QualMethod,ReportMethod

Data2=Filename2,filetext2,MSFile2,MsTuneFile2,InletFile2,InletPreRun2,INletPostRun2,InletSwitch2,AutoFile2,Process2,ProcessParam2,ProcessOptions2,SampleLocation2,Job2,Task2,User2,Submitter2,Conditions2,Analyte,ID2,-22,10.2,10.3,10.4,10.5,10.6,10.7,10.8,10.9,20.0,20.1,20.2,20.3,20.4,20.5,20.6,20.7,20.8,20.9,30.0,222.555,2.25,2.5,1.0,2.0,-22.5E-.2,32.12E+3,Spare12,Spare22,Spare32,Spare42,Spare52,QuantMethod2,QuantCalfile2,QualMethod2,ReportMethod2

Appendix F Environmental Reporting Calculations

About the Calculations

The calculation of compound concentration to be employed for a given sample will be determined by the analysis type (VOA or SV – taken from the ‘Analysis’ field in the sample list), matrix type (water/soil – taken from the ‘Matrix’ field in the sample list) and concentration level (low/medium – taken from the ‘Level’ field in the sample list).

This value calculated from the equations below will be included in the data source as the item under the TargetCompounds() collection (i.e. it will not replace the standard TurboMass ‘Concentration’ value found in the Quantify view results.

NOTE: *The equations below are shown in two forms. Firstly, the form defined in the EPA methods and/or SOW. The TurboMass software will not perform these calculations exactly as defined in these equations but will instead derive the ‘environmental concentrations’ from the concentration value currently calculated and reported. The secondary calculations required to generate the required ‘environmental concentration’ value from the current TurboMass concentration are defined in the equations shown in parenthesis [ ] following the EPA version.*

Volatile Organic Compound Analysis Water Samples

$$\text{Concentration}\,(\mu g/L) = \frac{(A_x)(I_s)(D_f)}{(A_{is})(\overline{RRF})(V_o)} \quad \left[\equiv \frac{(X_s)(D_f)}{(V_0)} \text{ (where Xs is TurboMass concentration}^{1}\text{)} \right]$$

where

A_x	Area[2] of the characteristic ion (Extracted Ion Current profile - EICP) for the compound to be measured – from integration results
A_{is}	Area of the characteristic ion (EICP) for the specific internal standard – from integration results
Is	Amount of internal standard added in nanograms (ng) – from appropriate Concentration column of the sample list (as defined in the Quantify Method and the sample list)
$\overline{RRF}$	Average relative response factor from the ambient temperature purge of the calibration standard – from calibration file
Vo	Volume of water purged in milliliters (mL) – 'Sample Vol' from sample list
Df	Dilution factor. The dilution factor for analysis of water samples for volatiles by this method is defined as the ratio of the number of milliliters (mL) of water purged (i.e., Vo above) to the number of mL of the original water sample used for purging) – from sample list (Dilution Factor) – 'Dilution Factor' from sample list)

NOTE: *For compounds designated as "Surrogate", the Concentration is calculated without including the Dilution Factor. This is because in Volatile Analysis the Surrogates are added following dilution and are therefore not affected by it. The equation (starting from TurboMass concentration) for Surrogates therefore becomes:*

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[1] X_s is the target concentration amount. This is calculated based on a concentration entered for the internal standard in the Sample List..

[2] "Area" is referenced here, since it is specified by the EPA methods, but the software will actually use whatever response mode (area or height) is specified in the Quantify Method. This applies to all the environmental calculation defined in this document.

$$\text{Concentration}\,(\mu\text{g/L}) = \frac{(X_s)}{(V_o)}$$

The average relative response factor ($\overline{RRF}$) is the average of the relative response factor values calculated at each calibration level:

$$\text{Relative reponse factor} = \frac{A_x}{A_{is}} \times \frac{C_{is}}{C_x}$$

where

A_x	Area of the characteristic ion (EICP) for the compound to be measured, in the calibration standard
A_{is}	Area of the characteristic ion (EICP) for the specific internal standard, in the calibration standard
C_{is}	Concentration of the internal standard in the calibration standard
C_x	Concentration of the compound to be measured, in the calibration standard

Soil/Sediment Samples (Low Level)

$$\text{Concentration}\,(\mu g/kg) = \frac{(A_x)\,(I_s)\,(D_f)}{(A_{is})\,(\overline{RRF})\,(W_s)\,(D)} \qquad \left[\equiv \frac{(X_s)\,(D_f)}{(W_s)(D)} \text{ (where Xs is TurboMass concentration}^{3}\text{)} \right]$$

where

A_x	Area of the characteristic ion (EICP) for the compound to be measured – from integration results
A_{is}	Area of the characteristic ion (EICP) for the specific internal standard – from integration results
I_s	Amount of internal standard added in nanograms (ng) – – from appropriate Concentration column of the sample list (as defined in the Quantify Method)
$\overline{RRF}$	Average relative response factor from the heated purge of the calibration standard – from calibration file
D	Adjustment for dry weight basis – (100 - %moisture)/100 – calculated from % Moisture value in sample list
W_s	Weight of sample added to the purge tube, in grams (g) – 'Sample Wt' from sample list
Df	Dilution factor. [This is not included in the EPA equation but is being included here for consistency and to avoid the need for special cases in the software.]

[3] X_s is the target concentration amount. This is calculated based on a concentration entered for the internal standard in the Sample List.

Soil/Sediment Samples (Medium Level)

$$\text{Concentration}\,(\mu g/kg) = \frac{(A_x)(I_s)(V_t)(1000)(D_f)}{(A_{is})(\overline{RRF})(V_a)(W_s)(D)} \quad \left[\equiv \frac{(X_s)(V_t)(1000)(D_f)}{(V_a)(W_s)(D)} \right.$$ (where Xs is TurboMass concentration[34] $\left. \right]$

)

where

A_x	Area of the characteristic ion (EICP) for the compound to be measured – from integration results
A_{is}	Area of the characteristic ion (EICP) for the specific internal standard – from integration results
I_s	Amount of internal standard added in nanograms (ng) – from appropriate Concentration column of the sample list (as defined in the Quantify Method)
$\overline{RRF}$	Average relative response factor from the heated purge of the calibration standard – from calibration file
V_t	Total volume of the methanol extract in milliliters (mL) – 'Soil Extract Volume' from sample list
V_a	Volume of the aliquot of the sample methanol extract (i.e., sample extract not including the methanol added to equal 100 µL) in microliters (µL) added to reagent water for purging – 'Soil Aliquot Volume' from sample list
W_s	Weight of soil/sediment extracted, in grams (g) – 'Sample Wt' from sample list
D	Adjustment for dry weight basis – (100 – %moisture)/ 100 – calculated from % Moisture value in sample list)
Df	Dilution factor. The dilution factor for analysis of soil/sediment samples for volatiles by the medium level method is defined as: [(µL most conc. extract used to make dilution) + (µL clean solvent)] / (µL most conc. extract used to make dilution)– from sample list (Dilution Factor) – 'Dilution Factor' from sample list

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[4] Xs is the target concentration amount. This is calculated based on a concentration entered for the internal standard in the Sample List.

NOTE: *For compounds designated as "Surrogate", the Concentration is calculated without including the Dilution Factor. This is because in Volatile Analysis the Surrogates are added following dilution and are therefore not affected by it. The equation (starting from TurboMass concentration) for Surrogates therefore becomes:*

$$\text{Concentration}\,(\mu g/Kg) = \frac{(X_s)(V_t)(1000)}{(V_a)(W_s)(D)}$$

The calculation for results of medium-and high-level soil/sediment volatile organic analyses preserved with methanol is in accordance with EPA SW-846, published Method 8000C, Revision 3, 03/03. Water contained in a sample mixes with the water-soluble methanol preservative to create a greater volume of liquid for analysis. To account for the dilution effect of the water to the methanol in the sample, a moisture adjustment must be applied. This will produce a more accurate quantitation on a sample specific basis for contaminates of concern. This moisture adjustment is not the same as reporting the data on a dry-weight basis. The data must also be adjusted to be reported on a dry weight basis.

NOTE: *This calculation will only be performed for Analysis=Volatiles, Matrix=Soil, Level=Medium (and if all required inputs are available).*

The total volume of methanol preservative and sample moisture contribution can be calculated as follows:

$$\text{Moisture} = \frac{\text{wt of sample - wt of dry sample}}{\text{wt of sample}} \quad \text{or} \quad \frac{(100 - \text{Sample \% solid})}{100}$$

$$V_t = V_e + (\text{Moisture} \times \text{wt of sample} \times 1000\mu L/mL)$$

where:

Moisture	The % Moisture value from the sample list expressed as a fraction (i.e. % Moisture/100)
V_t	Total volume of methanol plus water in the sample container for analysis
V_e	Total extract volume (usually assumed to be only the volume of methanol)

This adjusted value for Vt will then be used in the equation shown in section **Soil/Sediment Samples (Medium Level)**, in place of the nominal extract volume.

Semi-Volatile Organic Compound Analysis Water Samples

$$\text{Concentration}\,(\mu g/L) = \frac{(A_x)(I_s)(V_t)(D_f)(GPC)}{(A_{is})(\overline{RRF})(V_o)(V_i)} \left[\equiv \frac{(X_s)(V_t)(D_f)(GPC)}{(V_o)(V_i)} \;(\text{where Xs is TurboMass concentration}^{5})\right]$$

where

A_x	Area of the characteristic ion for the compound to be measured – from integration results
A_{is}	Area of the characteristic ion for the internal standard – from integration results
I_s	Amount of internal standard injected in nanograms (ng) – from appropriate Concentration column of the sample list (as defined in the Quantify Method)
V_o	Volume of water extracted in milliliters (mL) – 'Sample Vol' from sample list
V_i	Volume of extract injected in microliters (µL) – 'Injection Volume' from sample list
V_t	Volume of the concentrated extract in microliters (µL) – 'Concentrated Extract Volume' from sample list (If GPC is not performed, then Vt = 10,000 µL. If GPC is performed, then Vt = 5,000 µL.)
$\overline{RRF}$	Average relative response factor. – from calibration file
GPC	GPC factor – derived from setting in sample list (GPC Y/N) GPC = 1.0 if water sample was not subjected to GPC; GPC = 2.0 if water sample was subjected to GPC.
Df	Dilution factor. The dilution factor for analysis of water samples for semi-volatiles by this method is defined as follows: [(µL most conc. extract used to make dilution) + (µL clean solvent)] / (µL most conc. extract used to make dilution) – 'Dilution Factor' from sample list

The calculation applies to water low concentration and multi concentration. The low concentration calculation will not contain the GPC parameter.

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[5] X_s is the target amount in nanograms, which assumes that the internal standard amount is entered as nanograms in the Sample List. If the internal standard amount is entered as a concentration then the user must enter a user multiplier to make the necessary correction.

Soil Sediment Samples

$$\text{Concentration}\ (\mu g/kg) = \frac{(A_x)(I_s)(V_t)(D_f)(GPC)}{(A_{is})(\overline{RRF})(V_i)(W_s)(D)} \left[\equiv \frac{(X_s)(V_t)(D_f)(GPC)}{(V_i)(W_s)(D)} \text{ (where Xs is TurboMass concentration [6])} \right]$$

where

A_x	Area of the characteristic ion for the compound to be measured – from integration results
A_{is}	Area of the characteristic ion for the internal standard – from integration results
I_s	Amount of internal standard injected in nanograms (ng) – from appropriate Concentration column of the sample list (as defined in the Quantify Method)
V_t	Volume of the concentrated extract in microliters(µL) – 'Concentrated Extract Volume' from sample list)
V_i	Volume of the extract injected in microliters (µL) – 'Injection Volume' from sample list
W_s	Weight of sample extracted in grams (g) – 'Sample Wt' from sample list
GPC	GPC factor – derived from setting in sample list (GPC Y/N) GPC = 1.0 if water sample was not subjected to GPC; GPC = 2.0 if water sample was subjected to GPC.
$\overline{RRF}$	Average relative response factor – from calibration file
D	Adjustment for dry weight basis – (100 – %moisture)/100 – calculated from % moisture value in sample list Df Dilution factor. The dilution factor for analysis of soil/sediment samples for semi-volatiles by the medium level method is defined as follows: [(µL most conc. extract used to make dilution) + (µL clean solvent)] / (µL most conc. extract used to make dilution)

[6] X_s is the target amount in nanograms, which assumes that the internal standard amount is entered as nanograms in the Sample List. If the internal standard amount is entered as a concentration then the user must enter a user multiplier to make the necessary correction.

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